

Benzene, 1,1'-[4-(3-phenylpropyl)-1,7-heptanediyl]bis-

Other names:	1,7-Diphenyl-4-(3-phenylpropyl)heptane
Inchi:	InChI=1S/C28H34/c1-4-13-25(14-5-1)19-10-22-28(23-11-20-26-15-6-2-7-16-26)24-12-21
InchiKey:	QQEZQKPPCWXFPH-UHFFFAOYSA-N
Formula:	C28H34
SMILES:	c1ccc(CCCC(CCCc2ccccc2)CCc2ccccc2)cc1
Mol. weight [g/mol]:	370.57
CAS:	55282-64-9

Physical Properties

Property code	Value	Unit	Source
gf	519.67	kJ/mol	Joback Method
hf	83.06	kJ/mol	Joback Method
hfus	46.88	kJ/mol	Joback Method
hvap	84.36	kJ/mol	Joback Method
log10ws	-8.61		Crippen Method
logp	7.671		Crippen Method
mcvol	334.100	ml/mol	McGowan Method
pc	1184.97	kPa	Joback Method
tb	919.64	K	Joback Method
tc	1149.72	K	Joback Method
tf	469.58	K	Joback Method
vc	1.274	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1166.23	J/molxK	1149.72	Joback Method
cpg	1071.11	J/molxK	919.64	Joback Method
cpg	1089.84	J/molxK	957.99	Joback Method
cpg	1107.24	J/molxK	996.33	Joback Method
cpg	1123.44	J/molxK	1034.68	Joback Method
cpg	1138.59	J/molxK	1073.03	Joback Method
cpg	1152.80	J/molxK	1111.38	Joback Method
dvisc	0.0000326	Paxs	919.64	Joback Method

dvisc	0.0008126	Paxs	469.58	Joback Method
dvisc	0.0003288	Paxs	544.59	Joback Method
dvisc	0.0001656	Paxs	619.60	Joback Method
dvisc	0.0000967	Paxs	694.61	Joback Method
dvisc	0.0000627	Paxs	769.62	Joback Method
dvisc	0.0000440	Paxs	844.63	Joback Method
hvapt	100.30	kJ/mol	523.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.84581e+01
Coeff. B	-8.79586e+03
Coeff. C	-7.30340e+01
Temperature range (K), min.	557.11
Temperature range (K), max.	742.09

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55282649&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
h_{vapt}:	Enthalpy of vaporization at a given temperature
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
p_c:	Critical Pressure
p_{vap}:	Vapor pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/77-656-9/Benzene-1-1-4-3-phenylpropyl-1-7-heptanediyl-bis.pdf>

Generated by Cheméo on 2024-04-26 20:49:05.396204909 +0000 UTC m=+16453794.316782222.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.