

bis(2-ethylhexyl) benzene-1,4-dicarboxylate

Inchi:	InChI=1S/C24H38O4/c1-5-9-11-19(7-3)17-27-23(25)21-13-15-22(16-14-21)24(26)28-18-
InchiKey:	RWPICVVBGZBXNA-UHFFFAOYSA-N
Formula:	C24H38O4
SMILES:	CCCCC(CC)COC(=O)c1ccc(C(=O)OCC(CC)CCCC)cc1
Mol. weight [g/mol]:	390.56
CAS:	6422-86-2

Physical Properties

Property code	Value	Unit	Source
af	1.0534		Cheméo Relay (1.0)
hf	-953.46	kJ/mol	Cheméo Relay (1.0)
hfus	53.26	kJ/mol	Joback Method
hvap	112.00	kJ/mol	Cheméo Relay (1.0)
ie	9.21	eV	Cheméo Relay (1.0)
log10ws	-6.89		Cheméo Relay (1.0)
logp	6.433		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	988.88	kPa	Joback Method
tb	666.55	K	Cheméo Relay (1.0)
tc	860.90	K	Cheméo Relay (1.0)
tf	225.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)
vc	1.246	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	8.92000e+00
Coeff. B	2.04768e+00
Coeff. C	-1.06316e-03

Coeff. D	1.59800e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	$Y = \exp(A + B/T + C \cdot \ln(T) + D \cdot T^E)$
Y unit	Pa·s
Coeff. A	-1.46424e+01
Coeff. B	3.40752e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	225.15
Temperature range (K), max.	769.87

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
i_e:	Ionization energy
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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