Benzene, [3-(2-cyclohexylethyl)-6-cyclopentylhexyl]-

Other names: 1-Cyclohexyl-6-cyclopentyl-3-phenethylhexane
1-Phenyl-3-(2'-cyclohexylethyl)-6-cyclopentylhexane
Inchi: InChI=1S/C25H40/c1-3-10-23(11-4-1)18-20-25(17-9-16-22-14-7-8-15-22)21-19-24-12-5-2
InchiKey: DQHMQFJGANEDIX-UHFFFAOYSA-N
Formula: C25H40
SMILES: c1ccc(CCC(CCCC2CCCC2)CCC2CCCCC2)cc1
Mol. weight [g/mol]: 340.59
CAS: 55334-30-0

Physical Properties

Property code	Value	Unit	Source
gf	330.59	kJ/mol	Joback Method
hf	-213.28	kJ/mol	Joback Method
hfus	36.79	kJ/mol	Joback Method
hvap	73.82	kJ/mol	Joback Method
log10ws	-8.45		Crippen Method
logp	7.956		Crippen Method
mcvol	317.630	ml/mol	McGowan Method
pc	1194.00	kPa	Joback Method
tb	832.47	K	Joback Method
tc	1053.92	K	Joback Method
tf	401.21	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.94	J/mol×K	832.47	Joback Method
cpg	1167.56	J/mol×K	1017.01	Joback Method
cpg	1149.68	J/mol×K	980.11	Joback Method
cpg	1130.39	J/mol×K	943.20	Joback Method
cpg	1109.57	J/mol×K	906.29	Joback Method
cpg	1087.13	J/mol×K	869.38	Joback Method
cpg	1184.13	J/mol×K	1053.92	Joback Method

dvisc	0.0000729	Pa×s	832.47	Joback Method
dvisc	0.0000998	Pa×s	760.59	Joback Method
dvisc	0.0001460	Pa×s	688.72	Joback Method
dvisc	0.0002333	Pa×s	616.84	Joback Method
dvisc	0.0004219	Pa×s	544.96	Joback Method
dvisc	0.0009134	Pa×s	473.09	Joback Method
dvisc	0.0026083	Pa×s	401.21	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.88897e+01
Coeff. B	-9.76874e+03
Temperature range (K), min.	525.14
Temperature range (K), max.	719.44

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C55334300&Units=SI

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
hvap: Enthalpy of vaporization at standard conditions

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume