Cyclohexane, [6-cyclopentyl-3-(3-cyclopentylpropyl)hexyl]-

Other names: 1,7-Dicyclopentyl-4-(2'-cyclohexylethyl)heptane
4-(2-Cyclohexylethyl)-1,7-dicyclopentylheptane

Inchi: InChI=1S/C25H46/c1-2-10-24(11-3-1)20-21-25(18-8-16-22-12-4-5-13-22)19-9-17-23-14-

InchiKey: NSXDZWDBOGDTOY-UHFFFAOYSA-N

Formula: C25H46

SMILES: C1CCC(CCC(CCCC2CCCC2)CCCC2CCCC2)CC1

Mol. weight [g/mol]: 346.63

CAS: 55401-72-4

Physical Properties

Property code	Value	Unit	Source
gf	254.73	kJ/mol	Joback Method
hf	-389.33	kJ/mol	Joback Method
hfus	36.69	kJ/mol	Joback Method
hvap	71.80	kJ/mol	Joback Method
log10ws	-9.00		Crippen Method
logp	8.684		Crippen Method
mcvol	330.530	ml/mol	McGowan Method
pc	1078.51	kPa	Joback Method
tb	821.07	K	Joback Method
tc	1033.03	K	Joback Method
tf	385.69	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1144.33	J/mol×K	821.07	Joback Method
cpg	1170.84	J/mol×K	856.40	Joback Method
cpg	1195.57	J/mol×K	891.72	Joback Method
cpg	1218.61	J/mol×K	927.05	Joback Method
cpg	1240.08	J/mol×K	962.38	Joback Method
cpg	1260.06	J/mol×K	997.71	Joback Method
cpg	1278.66	J/mol×K	1033.03	Joback Method

dvisc	0.0040331	Pa×s	385.69	Joback Method
dvisc	0.0013597	Pa×s	458.25	Joback Method
dvisc	0.0006171	Pa×s	530.82	Joback Method
dvisc	0.0003386	Pa×s	603.38	Joback Method
dvisc	0.0002114	Pa×s	675.94	Joback Method
dvisc	0.0001446	Pa×s	748.51	Joback Method
dvisc	0.0001058	Pa×s	821.07	Joback Method
hvapt	88.80	kJ/mol	497.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.79193e+01
Coeff. B	-8.95688e+03
Coeff. C	-1.60720e+01
Temperature range (K), min.	524.07
Temperature range (K), max.	726.49

Sources

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=C55401724&Units=SI

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

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
hvapt:	Enthalpy of vaporization at a given temperature
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