Octadecane, 2,2,4,15,17,17-hexamethyl-7,12-bis(3,5,5-trimethyl

Other names: 2,2,4,15,17,17-Hexamethyl-7,12-di(3',5',5'-trimethylhexyl)octadecane
2,2,4,15,17,17-Hexamethyl-7,12-bis(3,5,5-trimethylhexyl)octadecane

Inchi: InChI=1S/C42H86/c1-33(29-39(5,6)7)21-25-37(26-22-34(2)30-40(8,9)10)19-17-18-20-38

InchiKey: ODRMXCPHVVYLHY-UHFFFAOYSA-N

Formula: C42H86

SMILES: CC(CCC(CCCCC(CCC(C)CC(C)(C)C)CCC(C)CC(C)(C)C)CCC(C)CC(C)(C)C)CC(C)(C)C

Mol. weight [g/mol]: 591.13

CAS: 55470-97-8

Physical Properties

Property code	Value	Unit	Source
gf	299.48	kJ/mol	Joback Method
hf	-976.89	kJ/mol	Joback Method
hfus	53.74	kJ/mol	Joback Method
hvap	101.57	kJ/mol	Joback Method
log10ws	-14.99		Crippen Method
logp	15.189		Crippen Method
mcvol	602.640	ml/mol	McGowan Method
pc	380.58	kPa	Joback Method
tb	1144.80	K	Joback Method
tc	1453.40	K	Joback Method
tf	482.78	K	Joback Method
vc	2.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2316.87	J/mol×K	1144.80	Joback Method
cpg	2356.19	J/mol×K	1196.23	Joback Method
cpg	2394.50	J/mol×K	1247.67	Joback Method
cpg	2432.41	J/mol×K	1299.10	Joback Method
cpg	2470.57	J/mol×K	1350.54	Joback Method
cpg	2509.61	J/mol×K	1401.97	Joback Method
cpg	2550.15	J/mol×K	1453.40	Joback Method

dvisc	0.0003857	Pa×s	482.78	Joback Method
dvisc	0.0000472	Pa×s	593.12	Joback Method
dvisc	0.0000111	Pa×s	703.45	Joback Method
dvisc	0.0000039	Pa×s	813.79	Joback Method
dvisc	0.0000018	Pa×s	924.13	Joback Method
dvisc	0.0000009	Pa×s	1034.46	Joback Method
dvisc	0.0000006	Pa×s	1144.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55470978&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume