

1,1,4,4,10,10,13,13-Octamethyl-cyclooctadecane

Inchi:	InChI=1S/C26H52/c1-23(2)15-11-9-12-17-25(5,6)21-22-26(7,8)18-14-10-13-16-24(3,4)20
InchiKey:	JNSFDAQIIASDIH-UHFFFAOYSA-N
Formula:	C26H52
SMILES:	CC1(C)CCCCC(C)(C)CCC(C)(C)CCCCC(C)(C)CC1
Mol. weight [g/mol]:	364.69
CAS:	23014-57-5

Physical Properties

Property code	Value	Unit	Source
gf	2.20	kJ/mol	Joback Method
hf	-599.63	kJ/mol	Joback Method
hfus	7.75	kJ/mol	Joback Method
hvap	70.43	kJ/mol	Joback Method
log10ws	-9.63		Crippen Method
logp	9.566		Crippen Method
mcvol	366.340	ml/mol	McGowan Method
pc	1022.04	kPa	Joback Method
tb	852.02	K	Joback Method
tc	1104.40	K	Joback Method
tf	438.00 ± 1.00	K	NIST Webbook
tf	438.00 ± 1.00	K	NIST Webbook
vc	1.317	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1274.30	J/mol×K	852.02	Joback Method
cpg	1314.59	J/mol×K	894.08	Joback Method
cpg	1354.73	J/mol×K	936.15	Joback Method
cpg	1395.18	J/mol×K	978.21	Joback Method
cpg	1436.41	J/mol×K	1020.27	Joback Method
cpg	1478.89	J/mol×K	1062.33	Joback Method
cpg	1523.10	J/mol×K	1104.40	Joback Method
hfust	20.17	kJ/mol	438.00	NIST Webbook

hfust	20.17	kJ/mol	438.20	NIST Webbook
sfust	46.40	J/mol×K	438.00	NIST Webbook

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=C23014575&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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