Heneicosane, 11-(2,2-dimethylpropyl)-

Other names: 11-(2',2'-Dimethylpropyl)heneicosane
11-Neopentylheneicosane
Inchi: InChI=1S/C26H54/c1-6-8-10-12-14-16-18-20-22-25(24-26(3,4)5)23-21-19-17-15-13-11-9
InchiKey: JOPYPDXSWNGCTB-UHFFFAOYSA-N
Formula: C26H54
SMILES: CCCCCCCCCCC(CCCCCCCCCC)CC(C)(C)C
Mol. weight [g/mol]: 366.71
CAS: 55282-10-5

Physical Properties

Property code	Value	Unit	Source
gf	168.44	kJ/mol	Joback Method
hf	-594.00	kJ/mol	Joback Method
hfus	52.16	kJ/mol	Joback Method
hvap	71.79	kJ/mol	Joback Method
log10ws	-10.22		Crippen Method
logp	10.100		Crippen Method
mcvol	377.200	ml/mol	McGowan Method
pc	735.62	kPa	Joback Method
tb	790.61	K	Joback Method
tc	968.98	K	Joback Method
tf	252.15	K	NIST Webbook
tf	252.20 ± 2.00	K	NIST Webbook
tf	252.20 ± 1.00	K	NIST Webbook
vc	1.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1344.16	J/mol×K	968.98	Joback Method
cpg	1217.16	J/mol×K	790.61	Joback Method
cpg	1241.03	J/mol×K	820.34	Joback Method
cpg	1263.74	J/mol×K	850.07	Joback Method
cpg	1285.35	J/mol×K	879.80	Joback Method

cpg	1305.92	J/mol×K	909.52	Joback Method
cpg	1325.50	J/mol×K	939.25	Joback Method
dvisc	0.0000324	Pa×s	790.61	Joback Method
dvisc	0.0025394	Pa×s	370.20	Joback Method
dvisc	0.0006882	Pa×s	440.27	Joback Method
dvisc	0.0002669	Pa×s	510.34	Joback Method
dvisc	0.0001301	Pa×s	580.40	Joback Method
dvisc	0.0000741	Pa×s	650.47	Joback Method
dvisc	0.0000470	Pa×s	720.54	Joback Method
hvapt	93.00	kJ/mol	493.50	NIST Webbook

Sources

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=C55282105&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
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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