13,21,25-Trimethyltripentacontane

Inchi: InChI=1S/C56H114/c1-6-8-10-12-14-16-18-19-20-21-22-23-24-25-26-27-28-29-30-31-32
InchiKey: GXOPJJNCCVVMDG-UHFFFAOYSA-N
Formula: C56H114
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CCCCCCCC(C)CCCCCCC
Mol. weight [g/mol]: 787.50

Physical Properties

Property code	Value	Unit	Source
gf	413.32	kJ/mol	Joback Method
hf	-1215.01	kJ/mol	Joback Method
hfus	130.23	kJ/mol	Joback Method
hvap	139.09	kJ/mol	Joback Method
log10ws	-22.54		Crippen Method
logp	21.659		Crippen Method
mcvol	799.900	ml/mol	McGowan Method
pc	231.67	kPa	Joback Method
rinpol	5363.00		NIST Webbook
rinpol	5363.00		NIST Webbook
tb	1479.36	K	Joback Method
tc	2842.55	K	Joback Method
tf	675.88	K	Joback Method
vc	3.154	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	3329.51	J/mol×K	1479.36	Joback Method
cpg	3480.83	J/mol×K	1706.56	Joback Method
cpg	3664.62	J/mol×K	1933.76	Joback Method
cpg	3926.88	J/mol×K	2160.95	Joback Method
cpg	4313.61	J/mol×K	2388.15	Joback Method
cpg	4870.80	J/mol×K	2615.35	Joback Method
cpg	5644.46	J/mol×K	2842.55	Joback Method
dvisc	0.0000228	Pa×s	675.88	Joback Method

dvisc	0.0000056	Pa×s	809.79	Joback Method
dvisc	0.0000021	Pa×s	943.71	Joback Method
dvisc	0.0000010	Pa×s	1077.62	Joback Method
dvisc	0.0000005	Pa×s	1211.53	Joback Method
dvisc	0.0000003	Pa×s	1345.45	Joback Method
dvisc	0.0000002	Pa×s	1479.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R337581&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume