13,21-Dimethyltripentacontane

Inchi: InChI=1S/C55H112/c1-5-7-9-11-13-15-17-18-19-20-21-22-23-24-25-26-27-28-29-30-31-3
InchiKey: MCDJTBAPKGLGCC-UHFFFAOYSA-N
Formula: C55H112
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)CCCCCCCC(C)CCCCCCCCCC
Mol. weight [g/mol]: 773.48

Physical Properties

Property code	Value	Unit	Source
gf	407.34	kJ/mol	Joback Method
hf	-1189.09	kJ/mol	Joback Method
hfus	131.16	kJ/mol	Joback Method
hvap	137.25	kJ/mol	Joback Method
log10ws	-22.36		Crippen Method
logp	21.413		Crippen Method
mcvol	785.810	ml/mol	McGowan Method
pc	238.00	kPa	Joback Method
rinpol	5341.00		NIST Webbook
tb	1456.92	K	Joback Method
tc	2733.79	K	Joback Method
tf	679.61	K	Joback Method
vc	3.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	3257.15	J/mol×K	1456.92	Joback Method
cpg	3396.91	J/mol×K	1669.73	Joback Method
cpg	3558.66	J/mol×K	1882.54	Joback Method
cpg	3779.55	J/mol×K	2095.36	Joback Method
cpg	4096.72	J/mol×K	2308.17	Joback Method
cpg	4547.31	J/mol×K	2520.98	Joback Method
cpg	5168.46	J/mol×K	2733.79	Joback Method
dvisc	0.0000245	Pa×s	679.61	Joback Method
dvisc	0.0000066	Pa×s	809.16	Joback Method

dvisc	0.0000026	Pa×s	938.71	Joback Method
dvisc	0.0000012	Pa×s	1068.26	Joback Method
dvisc	0.0000007	Pa×s	1197.82	Joback Method
dvisc	0.0000005	Pa×s	1327.37	Joback Method
dvisc	0.0000003	Pa×s	1456.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R337596&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