13,21,25-trimethylhenpentacontane

Inchi: InChI=1S/C54H110/c1-6-8-10-12-14-16-18-19-20-21-22-23-24-25-26-27-28-29-30-31-33
InchiKey: LRQDCTLDSBYWMV-UHFFFAOYSA-N
Formula: C54H110
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CCCCCCCC(C)CCCCCCCCC
Mol. weight [g/mol]: 759.45

Physical Properties

Property code	Value	Unit	Source
gf	396.48	kJ/mol	Joback Method
hf	-1173.73	kJ/mol	Joback Method
hfus	125.05	kJ/mol	Joback Method
hvap	134.63	kJ/mol	Joback Method
log10ws	-21.70		Crippen Method
logp	20.879		Crippen Method
mcvol	771.720	ml/mol	McGowan Method
pc	245.83	kPa	Joback Method
rinpol	5164.00		NIST Webbook
rinpol	5164.00		NIST Webbook
rinpol	5164.00		NIST Webbook
tb	1433.60	K	Joback Method
tc	2559.26	K	Joback Method
tf	653.34	K	Joback Method
vc	3.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	3181.80	J/mol×K	1433.60	Joback Method
cpg	3300.99	J/mol×K	1621.21	Joback Method
cpg	3430.05	J/mol×K	1808.82	Joback Method
cpg	3593.94	J/mol×K	1996.43	Joback Method
cpg	3817.60	J/mol×K	2184.04	Joback Method
cpg	4126.01	J/mol×K	2371.65	Joback Method
cpg	4544.12	J/mol×K	2559.26	Joback Method

dvisc	0.0000328	Pa×s	653.34	Joback Method
dvisc	0.0000081	Pa×s	783.38	Joback Method
dvisc	0.0000030	Pa×s	913.43	Joback Method
dvisc	0.0000014	Pa×s	1043.47	Joback Method
dvisc	0.0000008	Pa×s	1173.51	Joback Method
dvisc	0.0000005	Pa×s	1303.56	Joback Method
dvisc	0.0000003	Pa×s	1433.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R337338&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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