

13,23,27-trimethylhenpentacontane

Inchi:	InChI=1S/C54H110/c1-6-8-10-12-14-16-18-19-20-21-22-23-24-25-26-27-28-29-31-34-38
InchiKey:	MWNNWCCDYCXZEC-UHFFFAOYSA-N
Formula:	C54H110
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CCCCCCCC(C)CCCCCCCC
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
tb	1433.60	K	Joback Method
tc	2559.26	K	Joback Method
tf	653.34	K	Joback Method
vc	3.042	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	3181.80	J/molxK	1433.60	Joback Method
cpg	3300.99	J/molxK	1621.21	Joback Method
cpg	3430.05	J/molxK	1808.82	Joback Method
cpg	3593.94	J/molxK	1996.43	Joback Method
cpg	3817.60	J/molxK	2184.04	Joback Method
cpg	4126.01	J/molxK	2371.65	Joback Method
cpg	4544.12	J/molxK	2559.26	Joback Method
dvisc	0.0000328	Paxs	653.34	Joback Method
dvisc	0.0000081	Paxs	783.38	Joback Method

dvisc	0.0000030	Paxs	913.43	Joback Method
dvisc	0.0000014	Paxs	1043.47	Joback Method
dvisc	0.0000008	Paxs	1173.51	Joback Method
dvisc	0.0000005	Paxs	1303.56	Joback Method
dvisc	0.0000003	Paxs	1433.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R338168&Units=SI
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

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

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