

Tetracontane, 13,17-dimethyl

Inchi: InChI=1S/C42H86/c1-5-7-9-11-13-15-17-18-19-20-21-22-23-24-25-26-27-29-31-33-35-38
InchiKey: NRPYVYLIXSJHE-UHFFFAOYSA-N
Formula: C42H86
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CCCCCCCCCCCC
Mol. weight [g/mol]: 591.13

Physical Properties

Property code	Value	Unit	Source
gf	297.88	kJ/mol	Joback Method
hf	-920.77	kJ/mol	Joback Method
hfus	97.49	kJ/mol	Joback Method
hvap	108.31	kJ/mol	Joback Method
log10ws	-16.92		Crippen Method
logp	16.342		Crippen Method
mcvol	602.640	ml/mol	McGowan Method
pc	365.03	kPa	Joback Method
rinsol	4049.00		NIST Webbook
tb	1159.48	K	Joback Method
tc	1578.86	K	Joback Method
tf	533.10	K	Joback Method
vc	2.376	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2317.64	J/molxK	1159.48	Joback Method
cpg	2518.29	J/molxK	1508.96	Joback Method
cpg	2483.33	J/molxK	1439.06	Joback Method
cpg	2446.79	J/molxK	1369.17	Joback Method
cpg	2407.66	J/molxK	1299.27	Joback Method
cpg	2364.94	J/molxK	1229.38	Joback Method
cpg	2552.67	J/molxK	1578.86	Joback Method
dvisc	0.0000029	Paxs	1159.48	Joback Method
dvisc	0.0000042	Paxs	1055.08	Joback Method

dvisc	0.0000067	Paxs	950.69	Joback Method
dvisc	0.0000117	Paxs	846.29	Joback Method
dvisc	0.0000241	Paxs	741.89	Joback Method
dvisc	0.0000627	Paxs	637.50	Joback Method
dvisc	0.0002380	Paxs	533.10	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R584524&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
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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