13,21-dimethylheptatriacontane

Inchi: InChI=1S/C39H80/c1-5-7-9-11-13-15-17-18-20-23-27-31-35-39(4)37-33-29-25-21-24-28-
InchiKey: BDNZFJYVVXMFBV-UHFFFAOYSA-N
Formula: C39H80
SMILES: CCCCCCCCCCCCCCC(C)CCCCCCCCCC(C)CCCCCCCCCCCC
Mol. weight [g/mol]: 549.05

Physical Properties

Property code	Value	Unit	Source
gf	272.62	kJ/mol	Joback Method
hf	-858.85	kJ/mol	Joback Method
hfus	89.72	kJ/mol	Joback Method
hvap	101.63	kJ/mol	Joback Method
log10ws	-15.66		Crippen Method
logp	15.172		Crippen Method
mcvol	560.370	ml/mol	McGowan Method
pc	408.78	kPa	Joback Method
rinpol	3758.00		NIST Webbook
rinpol	3758.00		NIST Webbook
rinpol	3758.00		NIST Webbook
rinpol	3759.00		NIST Webbook
rinpol	3744.00		NIST Webbook
rinpol	3759.00		NIST Webbook
rinpol	3758.00		NIST Webbook
tb	1090.84	K	Joback Method
tc	1428.32	K	Joback Method
tf	499.29	K	Joback Method
vc	2.208	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2105.46	J/mol×K	1090.84	Joback Method
cpg	2145.37	J/mol×K	1147.09	Joback Method
cpg	2181.80	J/mol×K	1203.33	Joback Method

cpg	2215.23	J/mol×K	1259.58	Joback Method
cpg	2246.16	J/mol×K	1315.83	Joback Method
cpg	2275.06	J/mol×K	1372.07	Joback Method
cpg	2302.42	J/mol×K	1428.32	Joback Method
dvisc	0.0003958	Pa×s	499.29	Joback Method
dvisc	0.0001036	Pa×s	597.88	Joback Method
dvisc	0.0000396	Pa×s	696.47	Joback Method
dvisc	0.0000192	Pa×s	795.06	Joback Method
dvisc	0.0000110	Pa×s	893.66	Joback Method
dvisc	0.0000070	Pa×s	992.25	Joback Method
dvisc	0.0000048	Pa×s	1090.84	Joback Method

Sources

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=R337343&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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