heptapentacontane

Inchi: InChI=1S/C57H116/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-37-39-41-43-45
InchiKey: LKRIKFXSOWDANL-UHFFFAOYSA-N
Formula: C57H116
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 801.53
CAS: 5856-67-7

Physical Properties

Property code	Value	Unit	Source
gf	429.06	kJ/mol	Joback Method
hf	-1219.81	kJ/mol	Joback Method
hfus	143.39	kJ/mol	Joback Method
hvap	142.48	kJ/mol	Joback Method
log10ws	-23.68		Crippen Method
logp	22.482		Crippen Method
mcvol	813.990	ml/mol	McGowan Method
pc	223.43	kPa	Joback Method
tb	1503.56	K	Joback Method
tc	3169.75	K	Joback Method
tf	369.70 ± 3.00	K	NIST Webbook
vc	3.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	3410.01	J/mol×K	1503.56	Joback Method
cpg	3610.74	J/mol×K	1781.26	Joback Method
cpg	3886.71	J/mol×K	2058.96	Joback Method
cpg	4323.63	J/mol×K	2336.65	Joback Method
cpg	5007.22	J/mol×K	2614.35	Joback Method
cpg	6023.20	J/mol×K	2892.05	Joback Method
cpg	7457.28	J/mol×K	3169.75	Joback Method
dvisc	0.0000145	Pa×s	732.15	Joback Method
dvisc	0.0000045	Pa×s	860.72	Joback Method

dvisc	0.0000019	Pa×s	989.29	Joback Method
dvisc	0.0000010	Pa×s	1117.86	Joback Method
dvisc	0.0000006	Pa×s	1246.42	Joback Method
dvisc	0.0000004	Pa×s	1374.99	Joback Method
dvisc	0.0000003	Pa×s	1503.56	Joback Method
hvapt	158.90	kJ/mol	755.50	NIST Webbook

Sources

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=C5856677&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume