1-Pentatricosene

Inchi: InChI=1S/C35H70/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-34-32-30-28-26-
InchiKey: NOCIDIARFGFRSA-UHFFFAOYSA-N
Formula: C35H70
SMILES: C=CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 490.93

Physical Properties

Property code	Value	Unit	Source
gf	331.66	kJ/mol	Joback Method
hf	-640.30	kJ/mol	Joback Method
hfus	85.13	kJ/mol	Joback Method
hvap	92.83	kJ/mol	Joback Method
log10ws	-14.33		Crippen Method
logp	13.675		Crippen Method
mcvol	499.710	ml/mol	McGowan Method
pc	486.02	kPa	Joback Method
rinpol	2485.00		NIST Webbook
rinpol	2485.00		NIST Webbook
tb	996.88	K	Joback Method
tc	1260.26	K	Joback Method
tf	482.45	K	Joback Method
vc	1.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1794.09	J/mol×K	996.88	Joback Method
cpg	1826.90	J/mol×K	1040.78	Joback Method
cpg	1857.46	J/mol×K	1084.67	Joback Method
cpg	1885.99	J/mol×K	1128.57	Joback Method
cpg	1912.70	J/mol×K	1172.46	Joback Method
cpg	1937.81	J/mol×K	1216.36	Joback Method
cpg	1961.53	J/mol×K	1260.26	Joback Method
dvisc	0.0005344	Pa×s	482.45	Joback Method

dvisc	0.0001766	Pa×s	568.19	Joback Method
dvisc	0.0000780	Pa×s	653.93	Joback Method
dvisc	0.0000416	Pa×s	739.66	Joback Method
dvisc	0.0000253	Pa×s	825.40	Joback Method
dvisc	0.0000169	Pa×s	911.14	Joback Method
dvisc	0.0000121	Pa×s	996.88	Joback Method

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=R608581&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
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