5,5-Diethylheptacosane

Inchi: InChI=1S/C31H64/c1-5-9-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-28-30-3
InchiKey: TUCZZSPBTFUWLS-UHFFFAOYSA-N
Formula: C31H64
SMILES: CCCCCCCCCCCCCCCCCCCCCCCC(CC)(CC)CCCC
Mol. weight [g/mol]: 436.84

Physical Properties

Property code	Value	Unit	Source
gf	212.98	kJ/mol	Joback Method
hf	-691.92	kJ/mol	Joback Method
hfus	68.63	kJ/mol	Joback Method
hvap	83.30	kJ/mol	Joback Method
log10ws	-12.56		Crippen Method
logp	12.195		Crippen Method
mcvol	447.650	ml/mol	McGowan Method
pc	573.70	kPa	Joback Method
rinpol	3018.00		NIST Webbook
rinpol	3018.00		NIST Webbook
tb	905.45	K	Joback Method
tc	1115.61	K	Joback Method
tf	441.55	K	Joback Method
vc	1.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1549.19	J/mol×K	905.45	Joback Method
cpg	1576.74	J/mol×K	940.48	Joback Method
cpg	1602.76	J/mol×K	975.50	Joback Method
cpg	1627.37	J/mol×K	1010.53	Joback Method
cpg	1650.67	J/mol×K	1045.55	Joback Method
cpg	1672.78	J/mol×K	1080.58	Joback Method
cpg	1693.80	J/mol×K	1115.61	Joback Method
dvisc	0.0009056	Pa×s	441.55	Joback Method

dvisc	0.0002808	Pa×s	518.87	Joback Method
dvisc	0.0001180	Pa×s	596.18	Joback Method
dvisc	0.0000605	Pa×s	673.50	Joback Method
dvisc	0.0000356	Pa×s	750.82	Joback Method
dvisc	0.0000231	Pa×s	828.13	Joback Method
dvisc	0.0000162	Pa×s	905.45	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=R415473&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