Octadecane, 9,10-diethyl

Inchi: InChI=1S/C22H46/c1-5-9-11-13-15-17-19-21(7-3)22(8-4)20-18-16-14-12-10-6-2/h21-22H
InchiKey: AVZUSORDOHPBIA-UHFFFAOYSA-N
Formula: C22H46
SMILES: CCCCCCCCC(CC)C(CC)CCCCCCCC
Mol. weight [g/mol]: 310.60

Physical Properties

Property code	Value	Unit	Source
gf	129.48	kJ/mol	Joback Method
hf	-507.97	kJ/mol	Joback Method
hfus	45.69	kJ/mol	Joback Method
hvap	63.79	kJ/mol	Joback Method
log10ws	-8.55		Crippen Method
logp	8.540		Crippen Method
mcvol	320.840	ml/mol	McGowan Method
pc	910.53	kPa	Joback Method
tb	701.88	K	Joback Method
tc	868.08	K	Joback Method
tf	307.70	K	Joback Method
vc	1.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	962.75	J/mol×K	701.88	Joback Method
cpg	984.94	J/mol×K	729.58	Joback Method
cpg	1006.16	J/mol×K	757.28	Joback Method
cpg	1026.44	J/mol×K	784.98	Joback Method
cpg	1045.81	J/mol×K	812.68	Joback Method
cpg	1064.30	J/mol×K	840.38	Joback Method
cpg	1081.95	J/mol×K	868.08	Joback Method
dvisc	0.0057276	Pa×s	307.70	Joback Method
dvisc	0.0014050	Pa×s	373.40	Joback Method
dvisc	0.0005248	Pa×s	439.09	Joback Method

dvisc	0.0002533	Pa×s	504.79	Joback Method
dvisc	0.0001446	Pa×s	570.49	Joback Method
dvisc	0.0000927	Pa×s	636.18	Joback Method
dvisc	0.0000646	Pa×s	701.88	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=R9453&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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