Heptadecanol

Inchi: InChI=1S/C17H36O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18/h18H,2-17H2,1H3
InchiKey: GOQYKNQRPGWPLP-UHFFFAOYSA-N
Formula: C17H36O
SMILES: CCCCCCCCCCCCCCCCCO
Mol. weight [g/mol]: 256.47
CAS: 52783-44-5

Physical Properties

Property code	Value	Unit	Source
gf	-44.56	kJ/mol	Joback Method
hf	-546.44	kJ/mol	Joback Method
hfus	43.87	kJ/mol	Joback Method
hvap	70.11	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.850		Crippen Method
mcvol	256.260	ml/mol	McGowan Method
pc	1314.65	kPa	Joback Method
rinpol	1968.00		NIST Webbook
rinpol	1969.00		NIST Webbook
rinpol	1969.00		NIST Webbook
rinpol	1965.00		NIST Webbook
rinpol	1954.00		NIST Webbook
rinpol	1965.00		NIST Webbook
tb	680.54	K	Joback Method
tc	841.88	K	Joback Method
tf	342.17	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	749.49	J/mol×K	680.54	Joback Method
cpg	766.98	J/mol×K	707.43	Joback Method
cpg	783.74	J/mol×K	734.32	Joback Method

cpg	799.79	J/mol×K	761.21	Joback Method
cpg	815.16	J/mol×K	788.10	Joback Method
cpg	829.86	J/mol×K	814.99	Joback Method
cpg	843.94	J/mol×K	841.88	Joback Method
dvisc	0.0067109	Pa×s	342.17	Joback Method
dvisc	0.0014953	Pa×s	398.56	Joback Method
dvisc	0.0004834	Pa×s	454.96	Joback Method
dvisc	0.0002005	Pa×s	511.36	Joback Method
dvisc	0.0000990	Pa×s	567.75	Joback Method
dvisc	0.0000556	Pa×s	624.14	Joback Method
dvisc	0.0000343	Pa×s	680.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52783445&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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