

1-Chloro-heptadecanone-2

Inchi:	InChI=1S/C17H33ClO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-17(19)16-18/h2-16H2,1H3
InchiKey:	AHDGMFJASVYUIA-UHFFFAOYSA-N
Formula:	C17H33ClO
SMILES:	CCCCCCCCCCCCCCCC(=O)CCl
Mol. weight [g/mol]:	288.90
CAS:	23546-12-5

Physical Properties

Property code	Value	Unit	Source
gf	-48.59	kJ/mol	Joback Method
hf	-522.53	kJ/mol	Joback Method
hfus	45.58	kJ/mol	Joback Method
hvap	64.57	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	6.276		Crippen Method
mvol	264.200	ml/mol	McGowan Method
pc	1253.92	kPa	Joback Method
tb	679.66	K	Joback Method
tc	851.49	K	Joback Method
tf	361.20	K	Joback Method
vc	1.042	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.52	J/molxK	679.66	Joback Method
cpg	817.53	J/molxK	822.85	Joback Method
cpg	802.85	J/molxK	794.21	Joback Method
cpg	787.44	J/molxK	765.57	Joback Method
cpg	771.26	J/molxK	736.94	Joback Method
cpg	754.30	J/molxK	708.30	Joback Method
cpg	831.51	J/molxK	851.49	Joback Method
dvisc	0.0001262	Paxs	679.66	Joback Method
dvisc	0.0001687	Paxs	626.58	Joback Method

dvisc	0.0002379	Paxs	573.51	Joback Method
dvisc	0.0003600	Paxs	520.43	Joback Method
dvisc	0.0005984	Paxs	467.35	Joback Method
dvisc	0.0011330	Paxs	414.28	Joback Method
dvisc	0.0025880	Paxs	361.20	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C23546125&Units=SI

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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