2-chloroethyl heptadecanoate

Inchi: InChI=1S/C19H37ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19(21)22-18-17-20/h2-
InchiKey: JJQWFUVLGQCSAI-UHFFFAOYSA-N
Formula: C19H37ClO2
SMILES: CCCCCCCCCCCCCCCCC(=O)OCCCl
Mol. weight [g/mol]: 332.95

Physical Properties

Property code	Value	Unit	Source
gf	-136.75	kJ/mol	Joback Method
hf	-696.03	kJ/mol	Joback Method
hfus	51.95	kJ/mol	Joback Method
hvap	71.43	kJ/mol	Joback Method
log10ws	-6.79		Crippen Method
logp	6.640		Crippen Method
mcvol	298.250	ml/mol	McGowan Method
pc	1087.06	kPa	Joback Method
rinpol	2302.00		NIST Webbook
ripol	2791.00		NIST Webbook
ripol	2777.00		NIST Webbook
tb	747.84	K	Joback Method
tc	923.13	K	Joback Method
tf	405.97	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.28	J/mol×K	747.84	Joback Method
cpg	902.70	J/mol×K	777.05	Joback Method
cpg	920.22	J/mol×K	806.27	Joback Method
cpg	936.86	J/mol×K	835.48	Joback Method
cpg	952.65	J/mol×K	864.70	Joback Method
cpg	967.61	J/mol×K	893.91	Joback Method
cpg	981.77	J/mol×K	923.13	Joback Method

dvisc	0.0014368	Pa×s	405.97	Joback Method
dvisc	0.0006456	Pa×s	462.95	Joback Method
dvisc	0.0003456	Pa×s	519.93	Joback Method
dvisc	0.0002094	Pa×s	576.90	Joback Method
dvisc	0.0001388	Pa×s	633.88	Joback Method
dvisc	0.0000984	Pa×s	690.86	Joback Method
dvisc	0.0000736	Pa×s	747.84	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R30787&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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