

2-chloroethyl nonadecanoate

Inchi:	InChI=1S/C21H41ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21(23)24-20-19
InchiKey:	VFAIYIHBNLHQDJ-UHFFFAOYSA-N
Formula:	C21H41ClO2
SMILES:	CCCCCCCCCCCCCCCCC(=O)OCCCl
Mol. weight [g/mol]:	361.00

Physical Properties

Property code	Value	Unit	Source
gf	-119.91	kJ/mol	Joback Method
hf	-737.31	kJ/mol	Joback Method
hfus	57.13	kJ/mol	Joback Method
hvap	75.88	kJ/mol	Joback Method
log10ws	-7.63		Crippen Method
logp	7.420		Crippen Method
mcvol	326.430	ml/mol	McGowan Method
pc	961.48	kPa	Joback Method
ripol	2510.00		NIST Webbook
ripol	2513.00		NIST Webbook
ripol	2513.00		NIST Webbook
ripol	3003.00		NIST Webbook
ripol	2997.00		NIST Webbook
ripol	3003.00		NIST Webbook
ripol	2999.00		NIST Webbook
ripol	3009.00		NIST Webbook
ripol	2997.00		NIST Webbook
tb	793.60	K	Joback Method
tc	973.90	K	Joback Method
tf	428.51	K	Joback Method
vc	1.284	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1005.07	J/mol×K	793.60	Joback Method

cpg	1024.39	J/mol×K	823.65	Joback Method
cpg	1042.70	J/mol×K	853.70	Joback Method
cpg	1060.04	J/mol×K	883.75	Joback Method
cpg	1076.44	J/mol×K	913.80	Joback Method
cpg	1091.93	J/mol×K	943.85	Joback Method
cpg	1106.54	J/mol×K	973.90	Joback Method
dvisc	0.0011536	Paxs	428.51	Joback Method
dvisc	0.0005079	Paxs	489.36	Joback Method
dvisc	0.0002681	Paxs	550.21	Joback Method
dvisc	0.0001607	Paxs	611.05	Joback Method
dvisc	0.0001057	Paxs	671.90	Joback Method
dvisc	0.0000745	Paxs	732.75	Joback Method
dvisc	0.0000554	Paxs	793.60	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R30826&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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