

Adipic acid, 8-chlorooctyl isobutyl ester

Inchi:	InChI=1S/C18H33ClO4/c1-16(2)15-23-18(21)12-8-7-11-17(20)22-14-10-6-4-3-5-9-13-19
InchiKey:	MNXUVEYWINNEBR-UHFFFAOYSA-N
Formula:	C18H33ClO4
SMILES:	CC(C)COC(=O)CCCCC(=O)OCCCCCCCCCI
Mol. weight [g/mol]:	348.90

Physical Properties

Property code	Value	Unit	Source
gf	-381.53	kJ/mol	Joback Method
hf	-925.47	kJ/mol	Joback Method
hfus	48.62	kJ/mol	Joback Method
hvap	77.97	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	4.869		Crippen Method
mcvol	291.600	ml/mol	McGowan Method
pc	1203.12	kPa	Joback Method
rinpol	2413.00		NIST Webbook
rinpol	2413.00		NIST Webbook
tb	800.81	K	Joback Method
tc	986.70	K	Joback Method
tf	451.86	K	Joback Method
vc	1.135	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.59	J/molxK	800.81	Joback Method
cpg	898.22	J/molxK	831.79	Joback Method
cpg	913.87	J/molxK	862.77	Joback Method
cpg	928.56	J/molxK	893.75	Joback Method
cpg	942.30	J/molxK	924.73	Joback Method
cpg	955.10	J/molxK	955.71	Joback Method
cpg	966.99	J/molxK	986.70	Joback Method
dvisc	0.0009679	Paxs	451.86	Joback Method

dvisc	0.0004596	Paxs	510.02	Joback Method
dvisc	0.0002542	Paxs	568.18	Joback Method
dvisc	0.0001569	Paxs	626.34	Joback Method
dvisc	0.0001052	Paxs	684.49	Joback Method
dvisc	0.0000750	Paxs	742.65	Joback Method
dvisc	0.0000562	Paxs	800.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349757&Units=SI
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

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

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