

Succinic acid, 2-chloropropyl isobutyl ester

Inchi:	InChI=1S/C11H19ClO4/c1-8(2)6-15-10(13)4-5-11(14)16-7-9(3)12/h8-9H,4-7H2,1-3H3
InchiKey:	SLQQAJCFZLRKR-UHFFFAOYSA-N
Formula:	C11H19ClO4
SMILES:	CC(C)COC(=O)CCC(=O)OCC(C)Cl
Mol. weight [g/mol]:	250.72

Physical Properties

Property code	Value	Unit	Source
gf	-442.91	kJ/mol	Joback Method
hf	-786.27	kJ/mol	Joback Method
hfus	26.97	kJ/mol	Joback Method
hvap	62.00	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	2.136		Crippen Method
mvol	192.970	ml/mol	McGowan Method
pc	2060.49	kPa	Joback Method
rinpol	1590.00		NIST Webbook
rinpol	1590.00		NIST Webbook
tb	640.21	K	Joback Method
tc	829.30	K	Joback Method
tf	357.97	K	Joback Method
vc	0.737	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.59	J/molxK	640.21	Joback Method
cpg	556.56	J/molxK	797.78	Joback Method
cpg	545.53	J/molxK	766.27	Joback Method
cpg	533.81	J/molxK	734.75	Joback Method
cpg	521.42	J/molxK	703.24	Joback Method
cpg	508.34	J/molxK	671.72	Joback Method
cpg	566.92	J/molxK	829.30	Joback Method
dvisc	0.0001359	Paxs	640.21	Joback Method

dvisc	0.0001814	Paxs	593.17	Joback Method
dvisc	0.0002544	Paxs	546.13	Joback Method
dvisc	0.0003802	Paxs	499.09	Joback Method
dvisc	0.0006180	Paxs	452.05	Joback Method
dvisc	0.0011245	Paxs	405.01	Joback Method
dvisc	0.0023947	Paxs	357.97	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=U349370&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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