

Succinic acid, 3-chlorophenethyl isobutyl ester

Inchi:	InChI=1S/C16H21ClO4/c1-12(2)11-21-16(19)7-6-15(18)20-9-8-13-4-3-5-14(17)10-13/h3-
InchiKey:	NVMCBDFXQIAIMW-UHFFFAOYSA-N
Formula:	C16H21ClO4
SMILES:	CC(C)COC(=O)CCC(=O)OCCc1cccc(Cl)c1
Mol. weight [g/mol]:	312.79

Physical Properties

Property code	Value	Unit	Source
gf	-295.59	kJ/mol	Joback Method
hf	-659.13	kJ/mol	Joback Method
hfus	37.10	kJ/mol	Joback Method
hvap	76.46	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.405		Crippen Method
mvol	239.660	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
rinpol	2192.00		NIST Webbook
rinpol	2192.00		NIST Webbook
tb	786.71	K	Joback Method
tc	995.09	K	Joback Method
tf	468.26	K	Joback Method
vc	0.914	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.77	J/molxK	786.71	Joback Method
cpg	689.96	J/molxK	821.44	Joback Method
cpg	703.13	J/molxK	856.17	Joback Method
cpg	715.28	J/molxK	890.90	Joback Method
cpg	726.45	J/molxK	925.63	Joback Method
cpg	736.62	J/molxK	960.36	Joback Method
cpg	745.84	J/molxK	995.09	Joback Method
dvisc	0.0008164	Paxs	468.26	Joback Method

dvisc	0.0004495	Paxs	521.34	Joback Method
dvisc	0.0002763	Paxs	574.41	Joback Method
dvisc	0.0001845	Paxs	627.48	Joback Method
dvisc	0.0001311	Paxs	680.56	Joback Method
dvisc	0.0000980	Paxs	733.63	Joback Method
dvisc	0.0000761	Paxs	786.71	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=U381493&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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