

Succinic acid, phenethyl 2-chloroethyl ester

Inchi: InChI=1S/C14H17ClO4/c15-9-11-19-14(17)7-6-13(16)18-10-8-12-4-2-1-3-5-12/h1-5H,6-1
InchiKey: XDCGMUHMVGHNY-UHFFFAOYSA-N
Formula: C14H17ClO4
SMILES: O=C(CCC(=O)OCCc1ccccc1)OCCCl
Mol. weight [g/mol]: 284.74

Physical Properties

Property code	Value	Unit	Source
gf	-300.36	kJ/mol	Joback Method
hf	-601.10	kJ/mol	Joback Method
hfus	35.83	kJ/mol	Joback Method
hvap	71.73	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.334		Crippen Method
mvol	211.480	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	2155.00		NIST Webbook
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tb	736.41	K	Joback Method
tc	944.98	K	Joback Method
tf	448.20	K	Joback Method
vc	0.808	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.10	J/molxK	736.41	Joback Method
cpg	580.53	J/molxK	771.17	Joback Method
cpg	593.03	J/molxK	805.93	Joback Method
cpg	604.61	J/molxK	840.69	Joback Method
cpg	615.29	J/molxK	875.46	Joback Method
cpg	625.08	J/molxK	910.22	Joback Method
cpg	634.00	J/molxK	944.98	Joback Method
dvisc	0.0010134	Paxs	448.20	Joback Method

dvisc	0.0005818	Paxs	496.24	Joback Method
dvisc	0.0003683	Paxs	544.27	Joback Method
dvisc	0.0002511	Paxs	592.31	Joback Method
dvisc	0.0001814	Paxs	640.34	Joback Method
dvisc	0.0001371	Paxs	688.38	Joback Method
dvisc	0.0001074	Paxs	736.41	Joback Method

Sources

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=U358001&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	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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