

Succinic acid, 2-chlorophenyl 2-(dimethylamino)ethyl ester

Inchi: InChI=1S/C14H18ClNO4/c1-16(2)9-10-19-13(17)7-8-14(18)20-12-6-4-3-5-11(12)15/h3-6
InchiKey: INNHLFZQXYLMSS-UHFFFAOYSA-N
Formula: C14H18ClNO4
SMILES: CN(C)CCOC(=O)CCC(=O)Oc1ccccc1Cl
Mol. weight [g/mol]: 299.75

Physical Properties

Property code	Value	Unit	Source
gf	-199.21	kJ/mol	Joback Method
hf	-545.04	kJ/mol	Joback Method
hfus	38.46	kJ/mol	Joback Method
hvap	74.44	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.130		Crippen Method
mvol	221.460	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
rinpol	2168.00		NIST Webbook
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tb	753.83	K	Joback Method
tc	961.15	K	Joback Method
tf	493.19	K	Joback Method
vc	0.827	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	605.60	J/mol×K	753.83	Joback Method
cpg	619.06	J/mol×K	788.38	Joback Method
cpg	631.56	J/mol×K	822.94	Joback Method
cpg	643.13	J/mol×K	857.49	Joback Method
cpg	653.78	J/mol×K	892.04	Joback Method
cpg	663.54	J/mol×K	926.60	Joback Method
cpg	672.42	J/mol×K	961.15	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=U357550&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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