Succinic acid, 4-(chloromethyl)benzyl ethyl ester

Inchi: InChI=1S/C14H17ClO4/c1-2-18-13(16)7-8-14(17)19-10-12-5-3-11(9-15)4-6-12/h3-6H,2,7

InchiKey: ZCBUXBQODIAWMQ-UHFFFAOYSA-N

Formula: C14H17ClO4

SMILES: CCOC(=O)CCC(=O)OCc1ccc(CCl)cc1

Mol. weight [g/mol]: 284.74

Physical Properties

Property code	Value	Unit	Source
gf	-309.99	kJ/mol	Joback Method
hf	-612.57	kJ/mol	Joback Method
hfus	35.44	kJ/mol	Joback Method
hvap	72.39	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	2.812		Crippen Method
mcvol	211.480	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
rinpol	2124.00		NIST Webbook
rinpol	2124.00		NIST Webbook
tb	741.39	K	Joback Method
tc	950.76	K	Joback Method
tf	460.72	K	Joback Method
vc	0.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.99	J/mol×K	741.39	Joback Method
cpg	579.31	J/mol×K	776.28	Joback Method
cpg	591.71	J/mol×K	811.18	Joback Method
cpg	603.21	J/mol×K	846.07	Joback Method
cpg	613.81	J/mol×K	880.97	Joback Method
cpg	623.52	J/mol×K	915.86	Joback Method
cpg	632.35	J/mol×K	950.76	Joback Method
dvisc	0.0008524	Pa×s	460.72	Joback Method

dvisc	0.0005150	Pa×s	507.50	Joback Method
dvisc	0.0003387	Pa×s	554.28	Joback Method
dvisc	0.0002378	Pa×s	601.06	Joback Method
dvisc	0.0001757	Pa×s	647.83	Joback Method
dvisc	0.0001353	Pa×s	694.61	Joback Method
dvisc	0.0001076	Pa×s	741.39	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=U381041&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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