Succinic acid, 3-methylbut-2-yl (2-chlorocyclohexyl)methyl ester

Inchi: InChI=1S/C16H27ClO4/c1-11(2)12(3)21-16(19)9-8-15(18)20-10-13-6-4-5-7-14(13)17/h11

InchiKey: ZCGQEJODSGNIFP-UHFFFAOYSA-N

Formula: C16H27ClO4

SMILES: CC(C)C(C)OC(=O)CCC(=O)OCC1CCCCC1Cl

Mol. weight [g/mol]: 318.84

Physical Properties

Property code	Value	Unit	Source
gf	-384.07	kJ/mol	Joback Method
hf	-855.49	kJ/mol	Joback Method
hfus	32.83	kJ/mol	Joback Method
hvap	73.25	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.695		Crippen Method
mcvol	252.560	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	2199.00		NIST Webbook
rinpol	2199.00		NIST Webbook
tb	769.49	K	Joback Method
tc	975.05	K	Joback Method
tf	417.46	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.97	J/mol×K	769.49	Joback Method
cpg	841.36	J/mol×K	940.79	Joback Method
cpg	828.38	J/mol×K	906.53	Joback Method
cpg	814.17	J/mol×K	872.27	Joback Method
cpg	798.70	J/mol×K	838.01	Joback Method
cpg	781.97	J/mol×K	803.75	Joback Method
cpg	853.11	J/mol×K	975.05	Joback Method
dvisc	0.0000901	Pa×s	769.49	Joback Method

dvisc	0.0001201	Pa×s	710.82	Joback Method
dvisc	0.0001686	Pa×s	652.15	Joback Method
dvisc	0.0002529	Pa×s	593.48	Joback Method
dvisc	0.0004149	Pa×s	534.80	Joback Method
dvisc	0.0007688	Pa×s	476.13	Joback Method
dvisc	0.0016943	Pa×s	417.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391399&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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