

Succinic acid, dec-2-yl (2-chlorocyclohexyl)methyl ester

Inchi:	InChI=1S/C21H37ClO4/c1-3-4-5-6-7-8-11-17(2)26-21(24)15-14-20(23)25-16-18-12-9-10
InchiKey:	XREABIWDBIKIDO-UHFFFAOYSA-N
Formula:	C21H37ClO4
SMILES:	CCCCCCCCC(C)OC(=O)CCC(=O)OCC1CCCCC1Cl
Mol. weight [g/mol]:	388.97

Physical Properties

Property code	Value	Unit	Source
gf	-339.53	kJ/mol	Joback Method
hf	-953.41	kJ/mol	Joback Method
hfus	49.30	kJ/mol	Joback Method
hvap	84.77	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	5.790		Crippen Method
mvol	323.010	ml/mol	McGowan Method
pc	1111.85	kPa	Joback Method
rinpol	2725.00		NIST Webbook
rinpol	2725.00		NIST Webbook
tb	884.33	K	Joback Method
tc	1088.19	K	Joback Method
tf	488.81	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.55	J/molxK	884.33	Joback Method
cpg	1138.82	J/molxK	1054.22	Joback Method
cpg	1126.38	J/molxK	1020.24	Joback Method
cpg	1112.56	J/molxK	986.26	Joback Method
cpg	1097.33	J/molxK	952.28	Joback Method
cpg	1080.67	J/molxK	918.31	Joback Method
cpg	1149.90	J/molxK	1088.19	Joback Method
dvisc	0.0000483	Paxs	884.33	Joback Method

dvisc	0.0000641	Paxs	818.41	Joback Method
dvisc	0.0000894	Paxs	752.49	Joback Method
dvisc	0.0001329	Paxs	686.57	Joback Method
dvisc	0.0002151	Paxs	620.65	Joback Method
dvisc	0.0003901	Paxs	554.73	Joback Method
dvisc	0.0008310	Paxs	488.81	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=U391404&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

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