

Succinic acid, 2,2-dichloroethyl cis-4-methylcyclohexyl ester

Inchi: InChI=1S/C13H20Cl2O4/c1-9-2-4-10(5-3-9)19-13(17)7-6-12(16)18-8-11(14)15/h9-11H,2
InchiKey: HAQDXGYIRCJKEB-UHFFFAOYSA-N
Formula: C13H20Cl2O4
SMILES: CC1CCC(OC(=O)CCC(=O)OCC(Cl)Cl)CC1
Mol. weight [g/mol]: 311.20

Physical Properties

Property code	Value	Unit	Source
gf	-418.82	kJ/mol	Joback Method
hf	-804.03	kJ/mol	Joback Method
hfus	32.78	kJ/mol	Joback Method
hvap	71.35	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.235		Crippen Method
mcvol	222.530	ml/mol	McGowan Method
pc	1944.08	kPa	Joback Method
rinpol	2030.00		NIST Webbook
rinpol	2030.00		NIST Webbook
tb	738.72	K	Joback Method
tc	951.12	K	Joback Method
tf	428.57	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.22	J/molxK	738.72	Joback Method
cpg	691.40	J/molxK	915.72	Joback Method
cpg	680.06	J/molxK	880.32	Joback Method
cpg	667.57	J/molxK	844.92	Joback Method
cpg	653.93	J/molxK	809.52	Joback Method
cpg	639.15	J/molxK	774.12	Joback Method
cpg	701.62	J/molxK	951.12	Joback Method
dvisc	0.0001287	Paxs	738.72	Joback Method

dvisc	0.0001665	Paxs	687.03	Joback Method
dvisc	0.0002246	Paxs	635.34	Joback Method
dvisc	0.0003194	Paxs	583.64	Joback Method
dvisc	0.0004866	Paxs	531.95	Joback Method
dvisc	0.0008116	Paxs	480.26	Joback Method
dvisc	0.0015314	Paxs	428.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390057&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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