

Succinic acid, cyclohexylmethyl 2,6-dichlorophenyl ester

Inchi:	InChI=1S/C17H20Cl2O4/c18-13-7-4-8-14(19)17(13)23-16(21)10-9-15(20)22-11-12-5-2-1
InchiKey:	SPKXQYDWSVOOMW-UHFFFAOYSA-N
Formula:	C17H20Cl2O4
SMILES:	O=C(CCC(=O)Oc1c(Cl)cccc1Cl)OCC1CCCCC1
Mol. weight [g/mol]:	359.24

Physical Properties

Property code	Value	Unit	Source
gf	-281.84	kJ/mol	Joback Method
hf	-647.38	kJ/mol	Joback Method
hfus	38.85	kJ/mol	Joback Method
hvap	84.55	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.803		Crippen Method
mvol	255.130	ml/mol	McGowan Method
pc	1848.33	kPa	Joback Method
rinpol	2614.00		NIST Webbook
rinpol	2614.00		NIST Webbook
tb	871.99	K	Joback Method
tc	1104.60	K	Joback Method
tf	544.35	K	Joback Method
vc	0.959	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	748.31	J/molxK	871.99	Joback Method
cpg	803.12	J/molxK	1065.83	Joback Method
cpg	794.94	J/molxK	1027.06	Joback Method
cpg	785.39	J/molxK	988.30	Joback Method
cpg	774.46	J/molxK	949.53	Joback Method
cpg	762.10	J/molxK	910.76	Joback Method
cpg	809.96	J/molxK	1104.60	Joback Method
dvisc	0.0000656	Paxs	871.99	Joback Method

dvisc	0.0000829	Paxs	817.38	Joback Method
dvisc	0.0001082	Paxs	762.78	Joback Method
dvisc	0.0001472	Paxs	708.17	Joback Method
dvisc	0.0002109	Paxs	653.56	Joback Method
dvisc	0.0003225	Paxs	598.96	Joback Method
dvisc	0.0005372	Paxs	544.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389868&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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