

Succinic acid, 2,3-dichlorophenyl cis-hex-3-en-1-yl ester

Inchi: InChI=1S/C16H18Cl2O4/c1-2-3-4-5-11-21-14(19)9-10-15(20)22-13-8-6-7-12(17)16(13)18
InchiKey: VFFBYCFOVUHUGE-ARJAWSKDSA-N
Formula: C16H18Cl2O4
SMILES: CCC=CCCOC(=O)CCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]: 345.22

Physical Properties

Property code	Value	Unit	Source
gf	-234.49	kJ/mol	Joback Method
hf	-563.84	kJ/mol	Joback Method
hfus	44.63	kJ/mol	Joback Method
hvap	81.85	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.578		Crippen Method
mcvol	247.600	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpol	2500.00		NIST Webbook
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tb	833.72	K	Joback Method
tc	1049.62	K	Joback Method
tf	520.62	K	Joback Method
vc	0.950	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.16	J/molxK	833.72	Joback Method
cpg	724.35	J/molxK	1013.64	Joback Method
cpg	715.71	J/molxK	977.65	Joback Method
cpg	706.20	J/molxK	941.67	Joback Method
cpg	695.79	J/molxK	905.69	Joback Method
cpg	684.45	J/molxK	869.70	Joback Method
cpg	732.14	J/molxK	1049.62	Joback Method
dvisc	0.0000636	Paxs	833.72	Joback Method

dvisc	0.0000796	Paxs	781.54	Joback Method
dvisc	0.0001029	Paxs	729.35	Joback Method
dvisc	0.0001383	Paxs	677.17	Joback Method
dvisc	0.0001954	Paxs	624.99	Joback Method
dvisc	0.0002941	Paxs	572.80	Joback Method
dvisc	0.0004803	Paxs	520.62	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=U391090&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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