

Succinic acid, 2,3-dichlorophenyl trans-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-ONEGZZNKSA-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
mvol	247.600	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpol	2419.00		NIST Webbook
rinpol	2419.00		NIST Webbook
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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391122&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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