

Succinic acid, 2-methylpent-3-yl 2,4-dichlorophenyl ester

Inchi: InChI=1S/C16H20Cl2O4/c1-4-13(10(2)3)21-15(19)7-8-16(20)22-14-6-5-11(17)9-12(14)18
InchiKey: XUVXJJTPIUORE-UHFFFAOYSA-N
Formula: C16H20Cl2O4
SMILES: CCC(OC(=O)CCC(=O)Oc1ccc(Cl)cc1Cl)C(C)C
Mol. weight [g/mol]: 347.23

Physical Properties

Property code	Value	Unit	Source
gf	-319.59	kJ/mol	Joback Method
hf	-691.62	kJ/mol	Joback Method
hfus	37.38	kJ/mol	Joback Method
hvap	81.12	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.657		Crippen Method
mvol	251.900	ml/mol	McGowan Method
pc	1708.95	kPa	Joback Method
rinpol	2308.00		NIST Webbook
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tb	828.68	K	Joback Method
tc	1044.31	K	Joback Method
tf	495.70	K	Joback Method
vc	0.958	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.03	J/mol×K	828.68	Joback Method
cpg	713.11	J/mol×K	864.62	Joback Method
cpg	725.12	J/mol×K	900.56	Joback Method
cpg	736.06	J/mol×K	936.49	Joback Method
cpg	745.95	J/mol×K	972.43	Joback Method
cpg	754.80	J/mol×K	1008.37	Joback Method
cpg	762.63	J/mol×K	1044.31	Joback Method
dvisc	0.0006451	Paxs	495.70	Joback Method

dvisc	0.0003577	Paxs	551.20	Joback Method
dvisc	0.0002210	Paxs	606.69	Joback Method
dvisc	0.0001480	Paxs	662.19	Joback Method
dvisc	0.0001054	Paxs	717.69	Joback Method
dvisc	0.0000789	Paxs	773.18	Joback Method
dvisc	0.0000613	Paxs	828.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389782&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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