

Succinic acid, 3-methylbut-2-yl 2,6-dichlorophenyl ester

Inchi: InChI=1S/C15H18Cl2O4/c1-9(2)10(3)20-13(18)7-8-14(19)21-15-11(16)5-4-6-12(15)17/h
InchiKey: VJLYULWIMLVFFI-UHFFFAOYSA-N
Formula: C15H18Cl2O4
SMILES: CC(C)C(C)OC(=O)CCC(=O)Oc1c(Cl)cccc1Cl
Mol. weight [g/mol]: 333.21

Physical Properties

Property code	Value	Unit	Source
gf	-328.01	kJ/mol	Joback Method
hf	-670.98	kJ/mol	Joback Method
hfus	34.79	kJ/mol	Joback Method
hvap	78.89	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.267		Crippen Method
mcvol	237.810	ml/mol	McGowan Method
pc	1853.11	kPa	Joback Method
rinpol	2176.00		NIST Webbook
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tb	805.80	K	Joback Method
tc	1023.38	K	Joback Method
tf	484.43	K	Joback Method
vc	0.901	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.59	J/mol×K	805.80	Joback Method
cpg	657.41	J/mol×K	842.06	Joback Method
cpg	669.19	J/mol×K	878.33	Joback Method
cpg	679.94	J/mol×K	914.59	Joback Method
cpg	689.67	J/mol×K	950.85	Joback Method
cpg	698.39	J/mol×K	987.11	Joback Method
cpg	706.10	J/mol×K	1023.38	Joback Method
dvisc	0.0007126	Paxs	484.43	Joback Method

dvisc	0.0004001	Paxs	537.99	Joback Method
dvisc	0.0002494	Paxs	591.55	Joback Method
dvisc	0.0001682	Paxs	645.12	Joback Method
dvisc	0.0001204	Paxs	698.68	Joback Method
dvisc	0.0000905	Paxs	752.24	Joback Method
dvisc	0.0000706	Paxs	805.80	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=U389865&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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