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

Inchi: InChI=1S/C15H18Cl2O4/c1-9(2)10(3)20-14(18)6-7-15(19)21-13-5-4-11(16)8-12(13)17/h4
InchiKey: ZYQFTCQNAHKMOX-UHFFFAOYSA-N
Formula: C15H18Cl2O4
SMILES: CC(C)C(C)OC(=O)CCC(=O)Oc1ccc(Cl)cc1Cl
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	2225.00		NIST Webbook
rinpol	2225.00		NIST Webbook
tb	805.80	K	Joback Method
tc	1023.38	K	Joback Method
tf	484.43	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.59	J/mol×K	805.80	Joback Method
cpg	698.39	J/mol×K	987.11	Joback Method
cpg	689.67	J/mol×K	950.85	Joback Method
cpg	679.94	J/mol×K	914.59	Joback Method
cpg	669.19	J/mol×K	878.33	Joback Method
cpg	657.41	J/mol×K	842.06	Joback Method
cpg	706.10	J/mol×K	1023.38	Joback Method
dvisc	0.0000706	Pa×s	805.80	Joback Method

dvisc	0.0000905	Pa×s	752.24	Joback Method
dvisc	0.0001204	Pa×s	698.68	Joback Method
dvisc	0.0001682	Pa×s	645.12	Joback Method
dvisc	0.0002494	Pa×s	591.55	Joback Method
dvisc	0.0004001	Pa×s	537.99	Joback Method
dvisc	0.0007126	Pa×s	484.43	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=U389781&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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