Dimethylmalonic acid, butyl 2,5-dichlorophenyl ester

Inchi: InChI=1S/C15H18Cl2O4/c1-4-5-8-20-13(18)15(2,3)14(19)21-12-9-10(16)6-7-11(12)17/h6

InchiKey: LSGVYAHOPOTMOU-UHFFFAOYSA-N

Formula: C15H18Cl2O4

SMILES: CCCCOC(=O)C(C)(C)C(=O)Oc1cc(Cl)ccc1Cl

Mol. weight [g/mol]: 333.21

Physical Properties

Property code	Value	Unit	Source
gf	-320.29	kJ/mol	Joback Method
hf	-669.17	kJ/mol	Joback Method
hfus	34.42	kJ/mol	Joback Method
hvap	78.37	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.268		Crippen Method
mcvol	237.810	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinpol	2039.00		NIST Webbook
rinpol	2039.00		NIST Webbook
tb	803.45	K	Joback Method
tc	1023.67	K	Joback Method
tf	516.85	K	Joback Method
vc	0.902	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.24	J/mol×K	803.45	Joback Method
cpg	657.91	J/mol×K	840.15	Joback Method
cpg	669.56	J/mol×K	876.86	Joback Method
cpg	680.23	J/mol×K	913.56	Joback Method
cpg	689.94	J/mol×K	950.26	Joback Method
cpg	698.73	J/mol×K	986.97	Joback Method
cpg	706.62	J/mol×K	1023.67	Joback Method
dvisc	0.0005224	Pa×s	516.85	Joback Method

dvisc	0.0003211	Pa×s	564.62	Joback Method
dvisc	0.0002129	Pa×s	612.38	Joback Method
dvisc	0.0001498	Pa×s	660.15	Joback Method
dvisc	0.0001106	Pa×s	707.92	Joback Method
dvisc	0.0000848	Pa×s	755.68	Joback Method
dvisc	0.0000671	Pa×s	803.45	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=U363680&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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