Dimethylmalonic acid, butyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C15H17Cl3O4/c1-4-5-6-21-13(19)15(2,3)14(20)22-12-10(17)7-9(16)8-11(12)18

InchiKey: WKDWODBQRJVSHX-UHFFFAOYSA-N

Formula: C15H17Cl3O4

SMILES: CCCCOC(=O)C(C)(C)C(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 367.65

Physical Properties

Property code	Value	Unit	Source
gf	-341.85	kJ/mol	Joback Method
hf	-696.38	kJ/mol	Joback Method
hfus	38.23	kJ/mol	Joback Method
hvap	83.42	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	4.922		Crippen Method
mcvol	250.050	ml/mol	McGowan Method
pc	1777.34	kPa	Joback Method
rinpol	2168.00		NIST Webbook
rinpol	2168.00		NIST Webbook
tb	845.86	K	Joback Method
tc	1069.99	K	Joback Method
tf	559.29	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.15	J/mol×K	845.86	Joback Method
cpg	677.55	J/mol×K	883.22	Joback Method
cpg	687.95	J/mol×K	920.57	Joback Method
cpg	697.38	J/mol×K	957.93	Joback Method
cpg	705.86	J/mol×K	995.28	Joback Method
cpg	713.42	J/mol×K	1032.64	Joback Method
cpg	720.09	J/mol×K	1069.99	Joback Method
dvisc	0.0003780	Pa×s	559.29	Joback Method

dvisc	0.0002446	Pa×s	607.05	Joback Method
dvisc	0.0001687	Pa×s	654.81	Joback Method
dvisc	0.0001223	Pa×s	702.58	Joback Method
dvisc	0.0000924	Pa×s	750.34	Joback Method
dvisc	0.0000722	Pa×s	798.10	Joback Method
dvisc	0.0000580	Pa×s	845.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363647&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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