Dimethylmalonic acid, butyl 2,4-dichloro-6-formylphenyl ester

Inchi: InChI=1S/C16H18Cl2O5/c1-4-5-6-22-14(20)16(2,3)15(21)23-13-10(9-19)7-11(17)8-12(13

InchiKey: UUTYWDOINDULJK-UHFFFAOYSA-N

Formula: C16H18Cl2O5

SMILES: CCCCOC(=O)C(C)(C)C(=O)Oc1c(Cl)cc(Cl)cc1C=O

Mol. weight [g/mol]: 361.22

Physical Properties

Property code	Value	Unit	Source
gf	-421.02	kJ/mol	Joback Method
hf	-786.86	kJ/mol	Joback Method
hfus	38.91	kJ/mol	Joback Method
hvap	87.98	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.081		Crippen Method
mcvol	253.470	ml/mol	McGowan Method
pc	1800.03	kPa	Joback Method
rinpol	2241.00		NIST Webbook
rinpol	2241.00		NIST Webbook
tb	879.97	K	Joback Method
tc	1101.81	K	Joback Method
tf	582.64	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.01	J/mol×K	879.97	Joback Method
cpg	719.99	J/mol×K	916.94	Joback Method
cpg	729.95	J/mol×K	953.92	Joback Method
cpg	738.91	J/mol×K	990.89	Joback Method
cpg	746.89	J/mol×K	1027.86	Joback Method
cpg	753.93	J/mol×K	1064.83	Joback Method
cpg	760.06	J/mol×K	1101.81	Joback Method
dvisc	0.0004013	Pa×s	582.64	Joback Method

dvisc	0.0002606	Pa×s	632.19	Joback Method
dvisc	0.0001802	Pa×s	681.75	Joback Method
dvisc	0.0001310	Pa×s	731.31	Joback Method
dvisc	0.0000991	Pa×s	780.86	Joback Method
dvisc	0.0000776	Pa×s	830.41	Joback Method
dvisc	0.0000624	Pa×s	879.97	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=U363632&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