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

Inchi: InChI=1S/C18H22Cl2O5/c1-4-7-8-24-16(22)18(5-2,6-3)17(23)25-15-12(11-21)9-13(19)10

InchiKey: GQCDWRQKCLWLJV-UHFFFAOYSA-N

Formula: C18H22Cl2O5

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

Mol. weight [g/mol]: 389.27

Physical Properties

Property code	Value	Unit	Source
gf	-404.18	kJ/mol	Joback Method
hf	-828.14	kJ/mol	Joback Method
hfus	44.09	kJ/mol	Joback Method
hvap	92.43	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	4.861		Crippen Method
mcvol	281.650	ml/mol	McGowan Method
pc	1539.08	kPa	Joback Method
rinpol	2398.00		NIST Webbook
tb	925.73	K	Joback Method
tc	1146.53	K	Joback Method
tf	605.18	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.16	J/mol×K	925.73	Joback Method
cpg	833.61	J/mol×K	962.53	Joback Method
cpg	843.97	J/mol×K	999.33	Joback Method
cpg	853.27	J/mol×K	1036.13	Joback Method
cpg	861.54	J/mol×K	1072.93	Joback Method
cpg	868.83	J/mol×K	1109.73	Joback Method
cpg	875.16	J/mol×K	1146.53	Joback Method
dvisc	0.0003230	Pa×s	605.18	Joback Method
dvisc	0.0002048	Pa×s	658.61	Joback Method

dvisc	0.0001391	Pa×s	712.03	Joback Method
dvisc	0.0000997	Pa×s	765.46	Joback Method
dvisc	0.0000746	Pa×s	818.88	Joback Method
dvisc	0.0000579	Pa×s	872.31	Joback Method
dvisc	0.0000462	Pa×s	925.73	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=U370063&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

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