Dimethylmalonic acid, 2,5-dichlorophenyl heptyl ester

Inchi: InChI=1S/C18H24Cl2O4/c1-4-5-6-7-8-11-23-16(21)18(2,3)17(22)24-15-12-13(19)9-10-14

InchiKey: QQUJORWJPJCZEA-UHFFFAOYSA-N

Formula: C18H24Cl2O4

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

Mol. weight [g/mol]: 375.29

Physical Properties

Property code	Value	Unit	Source
gf	-295.03	kJ/mol	Joback Method
hf	-731.09	kJ/mol	Joback Method
hfus	42.19	kJ/mol	Joback Method
hvap	85.05	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	5.439		Crippen Method
mcvol	280.080	ml/mol	McGowan Method
pc	1470.23	kPa	Joback Method
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook
tb	872.09	K	Joback Method
tc	1087.50	K	Joback Method
tf	550.66	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.48	J/mol×K	872.09	Joback Method
cpg	870.07	J/mol×K	1051.60	Joback Method
cpg	860.77	J/mol×K	1015.70	Joback Method
cpg	850.50	J/mol×K	979.79	Joback Method
cpg	839.23	J/mol×K	943.89	Joback Method
cpg	826.90	J/mol×K	907.99	Joback Method
cpg	878.44	J/mol×K	1087.50	Joback Method
dvisc	0.0000430	Pa×s	872.09	Joback Method

dvisc	0.0000549	Pa×s	818.52	Joback Method
dvisc	0.0000725	Pa×s	764.95	Joback Method
dvisc	0.0000999	Pa×s	711.38	Joback Method
dvisc	0.0001450	Pa×s	657.80	Joback Method
dvisc	0.0002249	Pa×s	604.23	Joback Method
dvisc	0.0003800	Pa×s	550.66	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=U363684&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