Diethylmalonic acid, 4-chloro-3-methylphenyl isobutyl ester

Inchi: InChI=1S/C18H25ClO4/c1-6-18(7-2,16(20)22-11-12(3)4)17(21)23-14-8-9-15(19)13(5)10-

InchiKey: LBMGDNJWJDLEEJ-UHFFFAOYSA-N

Formula: C18H25ClO4

SMILES: CCC(CC)(C(=O)OCC(C)C)C(=O)Oc1ccc(Cl)c(C)c1

Mol. weight [g/mol]: 340.84

Physical Properties

Property code	Value	Unit	Source
gf	-285.54	kJ/mol	Joback Method
hf	-720.63	kJ/mol	Joback Method
hfus	34.47	kJ/mol	Joback Method
hvap	80.27	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.559		Crippen Method
mcvol	267.840	ml/mol	McGowan Method
pc	1522.31	kPa	Joback Method
rinpol	2109.00		NIST Webbook
tb	834.22	K	Joback Method
tc	1048.15	K	Joback Method
tf	505.74	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	789.28	J/mol×K	834.22	Joback Method
cpg	852.23	J/mol×K	1012.50	Joback Method
cpg	841.76	J/mol×K	976.84	Joback Method
cpg	830.27	J/mol×K	941.19	Joback Method
cpg	817.71	J/mol×K	905.53	Joback Method
cpg	804.06	J/mol×K	869.88	Joback Method
cpg	861.70	J/mol×K	1048.15	Joback Method
dvisc	0.0000462	Pa×s	834.22	Joback Method
dvisc	0.0000601	Pa×s	779.47	Joback Method

dvisc	0.0000814	Pa×s	724.73	Joback Method
dvisc	0.0001158	Pa×s	669.98	Joback Method
dvisc	0.0001752	Pa×s	615.23	Joback Method
dvisc	0.0002877	Pa×s	560.49	Joback Method
dvisc	0.0005258	Pa×s	505.74	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=U369912&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