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

Inchi: InChI=1S/C16H21ClO4/c1-5-16(6-2,14(18)20-7-3)15(19)21-12-8-9-13(17)11(4)10-12/h8-

InchiKey: RBSUHTKVPBQRHK-UHFFFAOYSA-N

Formula: C16H21ClO4

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

Mol. weight [g/mol]: 312.79

Physical Properties

Property code	Value	Unit	Source
gf	-299.94	kJ/mol	Joback Method
hf	-674.07	kJ/mol	Joback Method
hfus	32.82	kJ/mol	Joback Method
hvap	76.21	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.923		Crippen Method
mcvol	239.660	ml/mol	McGowan Method
pc	1766.90	kPa	Joback Method
rinpol	1978.00		NIST Webbook
rinpol	1978.00		NIST Webbook
tb	788.90	K	Joback Method
tc	1003.50	K	Joback Method
tf	498.20	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.00	J/mol×K	788.90	Joback Method
cpg	690.15	J/mol×K	824.67	Joback Method
cpg	703.26	J/mol×K	860.43	Joback Method
cpg	715.35	J/mol×K	896.20	Joback Method
cpg	726.45	J/mol×K	931.97	Joback Method
cpg	736.60	J/mol×K	967.74	Joback Method
cpg	745.82	J/mol×K	1003.50	Joback Method
dvisc	0.0005728	Pa×s	498.20	Joback Method

dvisc	0.0003422	Pa×s	546.65	Joback Method
dvisc	0.0002223	Pa×s	595.10	Joback Method
dvisc	0.0001541	Pa×s	643.55	Joback Method
dvisc	0.0001124	Pa×s	692.00	Joback Method
dvisc	0.0000855	Pa×s	740.45	Joback Method
dvisc	0.0000672	Pa×s	788.90	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=U369910&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