Dimethylmalonic acid, monochloride, phenyl ester

Inchi: InChI=1S/C11H11ClO3/c1-11(2,9(12)13)10(14)15-8-6-4-3-5-7-8/h3-7H,1-2H3
InchiKey: DWONEIVVVSPZEN-UHFFFAOYSA-N
Formula: C11H11ClO3
SMILES: CC(C)(C(=O)Cl)C(=O)Oc1ccccc1
Mol. weight [g/mol]: 226.66

Physical Properties

Property code	Value	Unit	Source
gf	-217.78	kJ/mol	Joback Method
hf	-415.71	kJ/mol	Joback Method
hfus	19.46	kJ/mol	Joback Method
hvap	61.35	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.384		Crippen Method
mcvol	163.340	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
rinpol	1461.00		NIST Webbook
tb	642.12	K	Joback Method
tc	875.68	K	Joback Method
tf	394.58	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.77	J/mol×K	642.12	Joback Method
cpg	445.38	J/mol×K	836.75	Joback Method
cpg	436.48	J/mol×K	797.82	Joback Method
cpg	426.72	J/mol×K	758.90	Joback Method
cpg	416.05	J/mol×K	719.97	Joback Method
cpg	404.42	J/mol×K	681.05	Joback Method
cpg	453.47	J/mol×K	875.68	Joback Method
dvisc	0.0001733	Pa×s	642.12	Joback Method
dvisc	0.0002241	Pa×s	600.86	Joback Method

dvisc	0.0003011	Pa×s	559.61	Joback Method
dvisc	0.0004239	Pa×s	518.35	Joback Method
dvisc	0.0006333	Pa×s	477.09	Joback Method
dvisc	0.0010207	Pa×s	435.84	Joback Method
dvisc	0.0018179	Pa×s	394.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361811&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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