Diethylmalonic acid, monochloride, 3-methylbenzyl ester

Inchi: InChI=1S/C15H19ClO3/c1-4-15(5-2,13(16)17)14(18)19-10-12-8-6-7-11(3)9-12/h6-9H,4-5

InchiKey: OBGBKKJGWIPFIC-UHFFFAOYSA-N

Formula: C15H19ClO3

SMILES: CCC(CC)(C(=O)Cl)C(=O)OCc1cccc(C)c1

Mol. weight [g/mol]: 282.76

Physical Properties

Property code	Value	Unit	Source
gf	-193.73	kJ/mol	Joback Method
hf	-509.74	kJ/mol	Joback Method
hfus	29.43	kJ/mol	Joback Method
hvap	70.91	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.610		Crippen Method
mcvol	219.700	ml/mol	McGowan Method
pc	1973.55	kPa	Joback Method
rinpol	1830.00		NIST Webbook
rinpol	1830.00		NIST Webbook
tb	738.62	K	Joback Method
tc	956.98	K	Joback Method
tf	452.18	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.69	J/mol×K	738.62	Joback Method
cpg	657.73	J/mol×K	920.59	Joback Method
cpg	647.19	J/mol×K	884.20	Joback Method
cpg	635.77	J/mol×K	847.80	Joback Method
cpg	623.41	J/mol×K	811.41	Joback Method
cpg	610.07	J/mol×K	775.01	Joback Method
cpg	667.44	J/mol×K	956.98	Joback Method
dvisc	0.0001020	Pa×s	738.62	Joback Method

dvisc	0.0001317	Pa×s	690.88	Joback Method
dvisc	0.0001766	Pa×s	643.14	Joback Method
dvisc	0.0002483	Pa×s	595.40	Joback Method
dvisc	0.0003703	Pa×s	547.66	Joback Method
dvisc	0.0005963	Pa×s	499.92	Joback Method
dvisc	0.0010616	Pa×s	452.18	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369320&Units=SI

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