Diethylmalonic acid, monochloride, phenethyl ester

Inchi: InChI=1S/C15H19ClO3/c1-3-15(4-2,13(16)17)14(18)19-11-10-12-8-6-5-7-9-12/h5-9H,3-4

InchiKey: QLTHBKHAZONEPU-UHFFFAOYSA-N

Formula: C15H19ClO3

SMILES: CCC(CC)(C(=O)Cl)C(=O)OCCc1ccccc1

Mol. weight [g/mol]: 282.76

Physical Properties

Property code	Value	Unit	Source
gf	-184.10	kJ/mol	Joback Method
hf	-498.27	kJ/mol	Joback Method
hfus	29.82	kJ/mol	Joback Method
hvap	70.25	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.344		Crippen Method
mcvol	219.700	ml/mol	McGowan Method
pc	2000.12	kPa	Joback Method
rinpol	1818.00		NIST Webbook
rinpol	1818.00		NIST Webbook
tb	733.64	K	Joback Method
tc	951.21	K	Joback Method
tf	439.66	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.73	J/mol×K	733.64	Joback Method
cpg	611.24	J/mol×K	769.90	Joback Method
cpg	624.68	J/mol×K	806.16	Joback Method
cpg	637.12	J/mol×K	842.43	Joback Method
cpg	648.62	J/mol×K	878.69	Joback Method
cpg	659.23	J/mol×K	914.95	Joback Method
cpg	669.00	J/mol×K	951.21	Joback Method
dvisc	0.0012896	Pa×s	439.66	Joback Method

dvisc	0.0006837	Pa×s	488.66	Joback Method
dvisc	0.0004069	Pa×s	537.65	Joback Method
dvisc	0.0002641	Pa×s	586.65	Joback Method
dvisc	0.0001832	Pa×s	635.65	Joback Method
dvisc	0.0001339	Pa×s	684.64	Joback Method
dvisc	0.0001021	Pa×s	733.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369562&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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