Ethylphenylmalonic acid diethyl ester

Other names: Diethyl ethylphenylmalonate
Propanedioic acid, ethylphenyl-, diethyl ester
Malonic acid, ethylphenyl-, diethyl ester
Inchi: InChI=1S/C15H20O4/c1-4-15(13(16)18-5-2,14(17)19-6-3)12-10-8-7-9-11-12/h7-11H,4-6H
InchiKey: PKRVDBARWFJWEB-UHFFFAOYSA-N
Formula: C15H20O4
SMILES: CCOC(=O)C(CC)(C(=O)OCC)c1ccccc1
Mol. weight [g/mol]: 264.32
CAS: 76-67-5

Physical Properties

Property code	Value	Unit	Source
gf	-277.17	kJ/mol	Joback Method
hf	-614.75	kJ/mol	Joback Method
hfus	26.81	kJ/mol	Joback Method
hvap	68.28	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.461		Crippen Method
mcvol	213.330	ml/mol	McGowan Method
pc	2036.39	kPa	Joback Method
tb	718.63	K	Joback Method
tc	930.98	K	Joback Method
tf	431.97	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.90	J/mol×K	718.63	Joback Method
cpg	612.22	J/mol×K	754.02	Joback Method
cpg	626.46	J/mol×K	789.41	Joback Method
cpg	639.68	J/mol×K	824.81	Joback Method
cpg	651.90	J/mol×K	860.20	Joback Method
cpg	663.17	J/mol×K	895.59	Joback Method

cpg	673.51	J/mol×K	930.98	Joback Method
dvisc	0.0010981	Pa×s	431.97	Joback Method
dvisc	0.0005847	Pa×s	479.75	Joback Method
dvisc	0.0003490	Pa×s	527.52	Joback Method
dvisc	0.0002270	Pa×s	575.30	Joback Method
dvisc	0.0001577	Pa×s	623.08	Joback Method
dvisc	0.0001154	Pa×s	670.85	Joback Method
dvisc	0.0000880	Pa×s	718.63	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=C76675&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume