Ethyl «beta»-methyl-«beta»-phenyl-glycolate

Inchi: InChI=1S/C11H14O3/c1-3-14-10(12)11(2,13)9-7-5-4-6-8-9/h4-8,13H,3H2,1-2H3
InchiKey: ZYBCQQMOAQEIKV-UHFFFAOYSA-N
Formula: C11H14O3
SMILES: CCOC(=O)C(C)(O)c1ccccc1
Mol. weight [g/mol]: 194.23

Physical Properties

Property code	Value	Unit	Source
gf	-213.75	kJ/mol	Joback Method
hf	-439.62	kJ/mol	Joback Method
hfus	17.75	kJ/mol	Joback Method
hvap	66.89	kJ/mol	Joback Method
log10ws	-1.82		Crippen Method
logp	1.457		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
rinpol	1490.00		NIST Webbook
rinpol	1489.90		NIST Webbook
ripol	2213.70		NIST Webbook
ripol	2218.10		NIST Webbook
ripol	2213.70		NIST Webbook
tb	643.00	K	Joback Method
tc	849.38	K	Joback Method
tf	375.55	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.35	J/mol×K	643.00	Joback Method
cpg	415.60	J/mol×K	677.40	Joback Method
cpg	427.03	J/mol×K	711.79	Joback Method
cpg	437.68	J/mol×K	746.19	Joback Method
cpg	447.59	J/mol×K	780.58	Joback Method

cpg	456.79	J/mol×K	814.98	Joback Method
cpg	465.34	J/mol×K	849.38	Joback Method
dvisc	0.0030876	Pa×s	375.55	Joback Method
dvisc	0.0010831	Pa×s	420.12	Joback Method
dvisc	0.0004645	Pa×s	464.70	Joback Method
dvisc	0.0002310	Pa×s	509.27	Joback Method
dvisc	0.0001286	Pa×s	553.85	Joback Method
dvisc	0.0000781	Pa×s	598.42	Joback Method
dvisc	0.0000508	Pa×s	643.00	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=R252658&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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