

ethyl methylphenyl glycidate 1

Inchi:

InChI=1S/C12H14O3/c1-2-14-12(13)11-10(15-11)8-9-6-4-3-5-7-9/h3-7,10-11H,2,8H2,1H

InchiKey:

VBLCHSPDSRPGCQ-UHFFFAOYSA-N

Formula:

C12H14O3

SMILES:

CCOC(=O)C1OC1Cc1ccccc1

Mol. weight [g/mol]:

206.24

Physical Properties

Property code	Value	Unit	Source
gf	-104.43	kJ/mol	Joback Method
hf	-378.82	kJ/mol	Joback Method
hfus	30.85	kJ/mol	Joback Method
hvap	57.85	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	1.560		Crippen Method
mcvol	158.630	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
rinpol	1412.90		NIST Webbook
ripol	2112.00		NIST Webbook
tb	605.95	K	Joback Method
tc	824.60	K	Joback Method
tf	363.85	K	Joback Method
vc	0.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.98	J/mol×K	605.95	Joback Method
cpg	427.52	J/mol×K	642.39	Joback Method
cpg	442.05	J/mol×K	678.83	Joback Method
cpg	455.61	J/mol×K	715.28	Joback Method
cpg	468.25	J/mol×K	751.72	Joback Method
cpg	480.01	J/mol×K	788.16	Joback Method
cpg	490.94	J/mol×K	824.60	Joback Method
dvisc	0.0020555	Pa×s	363.85	Joback Method

dvisc	0.0014368	Pa×s	404.20	Joback Method
dvisc	0.0010717	Pa×s	444.55	Joback Method
dvisc	0.0008394	Pa×s	484.90	Joback Method
dvisc	0.0006826	Pa×s	525.25	Joback Method
dvisc	0.0005717	Pa×s	565.60	Joback Method
dvisc	0.0004902	Pa×s	605.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R185523&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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