Butanoic acid, 2-methyl-, 4-methoxy-2-(3-methyloxiranyl)phenyl ester

Other names: 2-(1',2'-Epoxypropyl)-4-methoxyphenyl 2-methylbutanoate
Inchi: InChI=1S/C15H20O4/c1-5-9(2)15(16)19-13-7-6-11(17-4)8-12(13)14-10(3)18-14/h6-10,14
InchiKey: VXWVNVFBEJTTKA-UHFFFAOYSA-N
Formula: C15H20O4
SMILES: CCC(C)C(=O)Oc1ccc(OC)cc1C1OC1C
Mol. weight [g/mol]: 264.32
CAS: 97180-28-4

Physical Properties

Property code	Value	Unit	Source
gf	-205.87	kJ/mol	Joback Method
hf	-601.18	kJ/mol	Joback Method
hfus	35.51	kJ/mol	Joback Method
hvap	67.88	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.107		Crippen Method
mcvol	206.770	ml/mol	McGowan Method
pc	2007.30	kPa	Joback Method
rinpol	1898.60		NIST Webbook
rinpol	1882.00		NIST Webbook
rinpol	1898.60		NIST Webbook
tb	706.53	K	Joback Method
tc	918.17	K	Joback Method
tf	429.93	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.77	J/mol×K	706.53	Joback Method
cpg	610.23	J/mol×K	741.80	Joback Method
cpg	625.67	J/mol×K	777.08	Joback Method
cpg	640.11	J/mol×K	812.35	Joback Method
cpg	653.58	J/mol×K	847.62	Joback Method

cpg	666.08	J/mol×K	882.89	Joback Method
cpg	677.66	J/mol×K	918.17	Joback Method
dvisc	0.0013215	Pa×s	429.93	Joback Method
dvisc	0.0009122	Pa×s	476.03	Joback Method
dvisc	0.0006723	Pa×s	522.13	Joback Method
dvisc	0.0005207	Pa×s	568.23	Joback Method
dvisc	0.0004190	Pa×s	614.33	Joback Method
dvisc	0.0003475	Pa×s	660.43	Joback Method
dvisc	0.0002954	Pa×s	706.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97180284&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

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