m-Anisic acid, 3-methylbut-2-enyl ester

Inchi: InChI=1S/C13H16O3/c1-10(2)7-8-16-13(14)11-5-4-6-12(9-11)15-3/h4-7,9H,8H2,1-3H3
InchiKey: WKINRCWZWLOOIQ-UHFFFAOYSA-N
Formula: C13H16O3
SMILES: COc1cccc(C(=O)OCC=C(C)C)c1
Mol. weight [g/mol]: 220.26
CAS: 204454-03-5

Physical Properties

Property code	Value	Unit	Source
gf	-105.89	kJ/mol	Joback Method
hf	-356.18	kJ/mol	Joback Method
hfus	25.95	kJ/mol	Joback Method
hvap	59.07	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	2.818		Crippen Method
mcvol	179.280	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinpol	1745.80		NIST Webbook
tb	631.25	K	Joback Method
tc	844.74	K	Joback Method
tf	350.56	K	Joback Method
vc	0.678	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.06	J/mol×K	631.25	Joback Method
cpg	463.02	J/mol×K	666.83	Joback Method
cpg	477.11	J/mol×K	702.41	Joback Method
cpg	490.35	J/mol×K	738.00	Joback Method
cpg	502.76	J/mol×K	773.58	Joback Method
cpg	514.36	J/mol×K	809.16	Joback Method
cpg	525.17	J/mol×K	844.74	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=C204454035&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
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