4-Ethylbenzoic acid, 3-methylbut-2-enyl ester

Inchi: InChI=1S/C14H18O2/c1-4-12-5-7-13(8-6-12)14(15)16-10-9-11(2)3/h5-9H,4,10H2,1-3H3
InchiKey: GSCBZQNTZAPPKA-UHFFFAOYSA-N
Formula: C14H18O2
SMILES: CCc1ccc(C(=O)OCC=C(C)C)cc1
Mol. weight [g/mol]: 218.29

Physical Properties

Property code	Value	Unit	Source
gf	7.53	kJ/mol	Joback Method
hf	-244.60	kJ/mol	Joback Method
hfus	27.35	kJ/mol	Joback Method
hvap	58.89	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.372		Crippen Method
mcvol	187.500	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	1727.00		NIST Webbook
tb	631.71	K	Joback Method
tc	844.11	K	Joback Method
tf	339.60	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.60	J/mol×K	631.71	Joback Method
cpg	488.45	J/mol×K	667.11	Joback Method
cpg	503.37	J/mol×K	702.51	Joback Method
cpg	517.39	J/mol×K	737.91	Joback Method
cpg	530.53	J/mol×K	773.31	Joback Method
cpg	542.85	J/mol×K	808.71	Joback Method
cpg	554.38	J/mol×K	844.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292541&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
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