3-Methylbut-2-enoic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C13H16O2/c1-9(2)5-13(14)15-12-7-10(3)6-11(4)8-12/h5-8H,1-4H3
InchiKey: CKMAWQPCGMFBBW-UHFFFAOYSA-N
Formula: C13H16O2
SMILES: CC(C)=CC(=O)Oc1cc(C)cc(C)c1
Mol. weight [g/mol]: 204.26

Physical Properties

Property code	Value	Unit	Source
gf	-10.52	kJ/mol	Joback Method
hf	-235.43	kJ/mol	Joback Method
hfus	24.37	kJ/mol	Joback Method
hvap	57.33	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.175		Crippen Method
mcvol	173.410	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
rinpol	1568.00		NIST Webbook
rinpol	1568.00		NIST Webbook
tb	613.81	K	Joback Method
tc	830.76	K	Joback Method
tf	340.85	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.84	J/mol×K	613.81	Joback Method
cpg	436.90	J/mol×K	649.97	Joback Method
cpg	451.08	J/mol×K	686.13	Joback Method
cpg	464.43	J/mol×K	722.28	Joback Method
cpg	476.96	J/mol×K	758.44	Joback Method
cpg	488.71	J/mol×K	794.60	Joback Method
cpg	499.71	J/mol×K	830.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307594&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
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