2-Ethylbutyric acid, 4-acetylphenyl ester

Inchi: InChI=1S/C14H18O3/c1-4-11(5-2)14(16)17-13-8-6-12(7-9-13)10(3)15/h6-9,11H,4-5H2,1-
InchiKey: NQIPBYSVMZRHAH-UHFFFAOYSA-N
Formula: C14H18O3
SMILES: CCC(CC)C(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]: 234.29

Physical Properties

Property code	Value	Unit	Source
gf	-195.50	kJ/mol	Joback Method
hf	-469.89	kJ/mol	Joback Method
hfus	26.53	kJ/mol	Joback Method
hvap	65.21	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.231		Crippen Method
mcvol	193.370	ml/mol	McGowan Method
pc	2206.22	kPa	Joback Method
rinpol	1800.00		NIST Webbook
tb	681.10	K	Joback Method
tc	892.57	K	Joback Method
tf	393.57	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.98	J/mol×K	681.10	Joback Method
cpg	528.96	J/mol×K	716.35	Joback Method
cpg	543.00	J/mol×K	751.59	Joback Method
cpg	556.13	J/mol×K	786.84	Joback Method
cpg	568.35	J/mol×K	822.08	Joback Method
cpg	579.70	J/mol×K	857.33	Joback Method
cpg	590.19	J/mol×K	892.57	Joback Method
dvisc	0.0016074	Pa×s	393.57	Joback Method
dvisc	0.0008611	Pa×s	441.49	Joback Method

dvisc	0.0005213	Pa×s	489.41	Joback Method
dvisc	0.0003451	Pa×s	537.33	Joback Method
dvisc	0.0002444	Pa×s	585.26	Joback Method
dvisc	0.0001824	Pa×s	633.18	Joback Method
dvisc	0.0001419	Pa×s	681.10	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U370096&Units=SI

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