

2-Ethylbutyric acid, 2-acethylphenyl ester

Inchi:	InChI=1S/C14H18O3/c1-4-11(5-2)14(16)17-13-9-7-6-8-12(13)10(3)15/h6-9,11H,4-5H2,1
InchiKey:	ZJMPGKXUVXBPII-UHFFFAOYSA-N
Formula:	C14H18O3
SMILES:	CCC(CC)C(=O)Oc1ccccc1C(C)=O
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	1679.00		NIST Webbook
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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/molxK	681.10	Joback Method
cpg	579.70	J/molxK	857.33	Joback Method
cpg	568.35	J/molxK	822.08	Joback Method
cpg	556.13	J/molxK	786.84	Joback Method
cpg	543.00	J/molxK	751.59	Joback Method
cpg	528.96	J/molxK	716.35	Joback Method
cpg	590.19	J/molxK	892.57	Joback Method
dvisc	0.0001419	Paxs	681.10	Joback Method

dvisc	0.0001824	Paxs	633.18	Joback Method
dvisc	0.0002444	Paxs	585.26	Joback Method
dvisc	0.0003451	Paxs	537.33	Joback Method
dvisc	0.0005213	Paxs	489.41	Joback Method
dvisc	0.0008611	Paxs	441.49	Joback Method
dvisc	0.0016074	Paxs	393.57	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U370104&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

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