N-(4-ethylphenyl)acetamide

Inchi: InChI=1S/C10H13NO/c1-3-9-4-6-10(7-5-9)11-8(2)12/h4-7H,3H2,1-2H3,(H,11,12)
InchiKey: HOPWGOFWAPWHDS-UHFFFAOYSA-N
Formula: C10H13NO
SMILES: CCc1ccc(NC(C)=O)cc1
Mol. weight [g/mol]: 163.22
CAS: 3663-34-1

Physical Properties

Property code	Value	Unit	Source
gf	96.57	kJ/mol	Joback Method
hf	-83.78	kJ/mol	Joback Method
hfus	22.01	kJ/mol	Joback Method
hvap	53.97	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.207		Crippen Method
mcvol	139.550	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
tb	563.90	K	Joback Method
tc	780.09	K	Joback Method
tf	366.65 ± 1.00	K	NIST Webbook
tf	367.90 ± 3.00	K	NIST Webbook
tf	363.60 ± 4.00	K	NIST Webbook
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.52	J/mol×K	563.90	Joback Method
cpg	337.10	J/mol×K	599.93	Joback Method
cpg	349.85	J/mol×K	635.96	Joback Method
cpg	361.81	J/mol×K	672.00	Joback Method
cpg	373.02	J/mol×K	708.03	Joback Method
cpg	383.49	J/mol×K	744.06	Joback Method
cpg	393.26	J/mol×K	780.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3663341&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume