Phenylacetamide, N-ethyl-N-(3-methylphenyl)-

Inchi: InChI=1S/C17H19NO/c1-3-18(16-11-7-8-14(2)12-16)17(19)13-15-9-5-4-6-10-15/h4-12H,
InchiKey: LTEOWCTWEIPQJP-UHFFFAOYSA-N
Formula: C17H19NO
SMILES: CCN(C(=O)Cc1ccccc1)c1cccc(C)c1
Mol. weight [g/mol]: 253.34

Physical Properties

Property code	Value	Unit	Source
gf	289.31	kJ/mol	Joback Method
hf	22.33	kJ/mol	Joback Method
hfus	32.10	kJ/mol	Joback Method
hvap	67.44	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.591		Crippen Method
mcvol	214.420	ml/mol	McGowan Method
pc	2179.52	kPa	Joback Method
rinpol	1965.00		NIST Webbook
rinpol	1965.00		NIST Webbook
tb	713.01	K	Joback Method
tc	942.10	K	Joback Method
tf	429.11	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.86	J/mol×K	713.01	Joback Method
cpg	600.75	J/mol×K	751.19	Joback Method
cpg	616.37	J/mol×K	789.37	Joback Method
cpg	630.80	J/mol×K	827.56	Joback Method
cpg	644.12	J/mol×K	865.74	Joback Method
cpg	656.41	J/mol×K	903.92	Joback Method
cpg	667.75	J/mol×K	942.10	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=U308407&Units=SI

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