Acetamide, N-[2,4-bis(1,1-dimethylethyl)phenyl]-

Other names: Acetanilide, 2,4-di-tert-butyl-
Inchi: InChI=1S/C16H25NO/c1-11(18)17-14-9-8-12(15(2,3)4)10-13(14)16(5,6)7/h8-10H,1-7H3,
InchiKey: TZFVZDNVBBQUGM-UHFFFAOYSA-N
Formula: C16H25NO
SMILES: CC(=O)Nc1ccc(C(C)(C)C)cc1C(C)(C)C
Mol. weight [g/mol]: 247.38
CAS: 38896-23-0

Physical Properties

Property code	Value	Unit	Source
gf	143.14	kJ/mol	Joback Method
hf	-236.59	kJ/mol	Joback Method
hfus	22.33	kJ/mol	Joback Method
hvap	65.40	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	4.240		Crippen Method
mcvol	224.090	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
tb	699.70	K	Joback Method
tc	918.97	K	Joback Method
tf	428.97	K	Joback Method
vc	0.843	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.69	J/mol×K	699.70	Joback Method
cpg	651.45	J/mol×K	736.25	Joback Method
cpg	667.99	J/mol×K	772.79	Joback Method
cpg	683.41	J/mol×K	809.34	Joback Method
cpg	697.79	J/mol×K	845.88	Joback Method
cpg	711.22	J/mol×K	882.43	Joback Method
cpg	723.79	J/mol×K	918.97	Joback Method

Sources

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=C38896230&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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