Acetamide, N-(3-methylphenyl)-2-phenyl-

Inchi: InChI=1S/C15H15NO/c1-12-6-5-9-14(10-12)16-15(17)11-13-7-3-2-4-8-13/h2-10H,11H2,1
InchiKey: XIZNMZFOCKTOLH-UHFFFAOYSA-N
Formula: C15H15NO
SMILES: Cc1cccc(NC(=O)Cc2ccccc2)c1
Mol. weight [g/mol]: 225.29

Physical Properties

Property code	Value	Unit	Source
gf	251.08	kJ/mol	Joback Method
hf	49.55	kJ/mol	Joback Method
hfus	29.00	kJ/mol	Joback Method
hvap	67.38	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.176		Crippen Method
mcvol	186.240	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
rinpol	2046.00		NIST Webbook
rinpol	2046.00		NIST Webbook
tb	704.98	K	Joback Method
tc	944.48	K	Joback Method
tf	426.76	K	Joback Method
vc	0.701	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.97	J/mol×K	704.98	Joback Method
cpg	507.21	J/mol×K	744.90	Joback Method
cpg	521.23	J/mol×K	784.81	Joback Method
cpg	534.11	J/mol×K	824.73	Joback Method
cpg	545.92	J/mol×K	864.65	Joback Method
cpg	556.74	J/mol×K	904.56	Joback Method
cpg	566.63	J/mol×K	944.48	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=U307142&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume