Benzamide, N-(3-methylphenyl)-2-methyl-

Inchi: InChI=1S/C15H15NO/c1-11-6-5-8-13(10-11)16-15(17)14-9-4-3-7-12(14)2/h3-10H,1-2H3,
InchiKey: UEOKUJAEEOJMST-UHFFFAOYSA-N
Formula: C15H15NO
SMILES: Cc1cccc(NC(=O)c2ccccc2C)c1
Mol. weight [g/mol]: 225.29

Physical Properties

Property code	Value	Unit	Source
gf	241.45	kJ/mol	Joback Method
hf	38.08	kJ/mol	Joback Method
hfus	28.61	kJ/mol	Joback Method
hvap	68.04	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.556		Crippen Method
mcvol	186.240	ml/mol	McGowan Method
pc	2629.85	kPa	Joback Method
rinpol	2049.00		NIST Webbook
tb	709.96	K	Joback Method
tc	950.27	K	Joback Method
tf	439.28	K	Joback Method
vc	0.701	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.89	J/mol×K	709.96	Joback Method
cpg	505.97	J/mol×K	750.01	Joback Method
cpg	519.86	J/mol×K	790.06	Joback Method
cpg	532.64	J/mol×K	830.12	Joback Method
cpg	544.37	J/mol×K	870.17	Joback Method
cpg	555.12	J/mol×K	910.22	Joback Method
cpg	564.95	J/mol×K	950.27	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=U307003&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