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
hf	-40.79	kJ/mol	Cheméo Relay (1.0)
hfus	28.61	kJ/mol	Joback Method
hvap	91.66	kJ/mol	Cheméo Relay (1.0)
ie	7.96	eV	Cheméo Relay (1.0)
log10ws	-4.25		Cheméo Relay (1.0)
logp	3.556		Crippen Method
mcvol	186.240	ml/mol	McGowan Method
rinpol	2049.00		NIST Webbook
tb	620.45	K	Cheméo Relay (1.0)
tc	927.22	K	Cheméo Relay (1.0)
tf	393.65	K	Cheméo Relay (1.0)

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307003&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point