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

Inchi: InChI=1S/C14H12BrNO/c1-10-5-4-6-11(9-10)16-14(17)12-7-2-3-8-13(12)15/h2-9H,1H3,(
InchiKey: XDQOOOIXHDTVLH-UHFFFAOYSA-N
Formula: C14H12BrNO
SMILES: Cc1cccc(NC(=O)c2ccccc2Br)c1
Mol. weight [g/mol]: 290.15

Physical Properties

Property code	Value	Unit	Source
gf	247.35	kJ/mol	Joback Method
hf	85.05	kJ/mol	Joback Method
hfus	31.30	kJ/mol	Joback Method
hvap	72.25	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.010		Crippen Method
mcvol	189.650	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
rinpol	2225.00		NIST Webbook
tb	753.24	K	Joback Method
tc	1008.78	K	Joback Method
tf	487.81	K	Joback Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.27	J/mol×K	753.24	Joback Method
cpg	486.07	J/mol×K	795.83	Joback Method
cpg	497.75	J/mol×K	838.42	Joback Method
cpg	508.40	J/mol×K	881.01	Joback Method
cpg	518.11	J/mol×K	923.60	Joback Method
cpg	526.97	J/mol×K	966.19	Joback Method
cpg	535.06	J/mol×K	1008.78	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=U307385&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

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