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

Inchi: InChI=1S/C9H10BrNO/c1-7-3-2-4-8(5-7)11-9(12)6-10/h2-5H,6H2,1H3,(H,11,12)
InchiKey: FSQVBULEPAWPNF-UHFFFAOYSA-N
Formula: C9H10BrNO
SMILES: Cc1cccc(NC(=O)CBr)c1
Mol. weight [g/mol]: 228.09

Physical Properties

Property code	Value	Unit	Source
gf	102.47	kJ/mol	Joback Method
hf	-36.81	kJ/mol	Joback Method
hfus	24.70	kJ/mol	Joback Method
hvap	58.18	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.328		Crippen Method
mcvol	142.960	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
rinpol	1622.00		NIST Webbook
rinpol	1622.00		NIST Webbook
tb	607.18	K	Joback Method
tc	840.54	K	Joback Method
tf	392.52	K	Joback Method
vc	0.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.03	J/mol×K	607.18	Joback Method
cpg	324.57	J/mol×K	646.07	Joback Method
cpg	335.27	J/mol×K	684.97	Joback Method
cpg	345.19	J/mol×K	723.86	Joback Method
cpg	354.37	J/mol×K	762.75	Joback Method
cpg	362.85	J/mol×K	801.64	Joback Method
cpg	370.69	J/mol×K	840.54	Joback Method

Sources

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=U307419&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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