Propanamide, N-ethyl-N-(3-methylphenyl)-2-bromo-

Inchi: InChI=1S/C12H16BrNO/c1-4-14(12(15)10(3)13)11-7-5-6-9(2)8-11/h5-8,10H,4H2,1-3H3
InchiKey: GZVOTXLLNZDDPZ-UHFFFAOYSA-N
Formula: C12H16BrNO
SMILES: CCN(C(=O)C(C)Br)c1cccc(C)c1
Mol. weight [g/mol]: 270.17

Physical Properties

Property code	Value	Unit	Source
gf	146.68	kJ/mol	Joback Method
hf	-89.95	kJ/mol	Joback Method
hfus	26.87	kJ/mol	Joback Method
hvap	60.08	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.131		Crippen Method
mcvol	185.230	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
rinpol	1665.00		NIST Webbook
rinpol	1665.00		NIST Webbook
tb	637.65	K	Joback Method
tc	860.51	K	Joback Method
tf	391.14	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.60	J/mol×K	637.65	Joback Method
cpg	461.34	J/mol×K	674.79	Joback Method
cpg	475.06	J/mol×K	711.94	Joback Method
cpg	487.82	J/mol×K	749.08	Joback Method
cpg	499.68	J/mol×K	786.22	Joback Method
cpg	510.71	J/mol×K	823.36	Joback Method
cpg	520.95	J/mol×K	860.51	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U308372&Units=SI

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