Hexanamide, N-ethyl-N-(3-methylphenyl)-6-bromo-

Inchi: InChI=1S/C15H22BrNO/c1-3-17(14-9-7-8-13(2)12-14)15(18)10-5-4-6-11-16/h7-9,12H,3-6

InchiKey: VFELMRDRJKSPMS-UHFFFAOYSA-N

Formula: C15H22BrNO

SMILES: CCN(C(=O)CCCCCBr)c1cccc(C)c1

Mol. weight [g/mol]: 312.25

Physical Properties

Property code	Value	Unit	Source
gf	174.38	kJ/mol	Joback Method
hf	-146.59	kJ/mol	Joback Method
hfus	38.16	kJ/mol	Joback Method
hvap	67.15	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	4.303		Crippen Method
mcvol	227.500	ml/mol	McGowan Method
pc	2043.76	kPa	Joback Method
rinpol	2026.00		NIST Webbook
tb	706.73	K	Joback Method
tc	915.27	K	Joback Method
tf	439.95	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.25	J/mol×K	706.73	Joback Method
cpg	617.96	J/mol×K	741.49	Joback Method
cpg	632.69	J/mol×K	776.24	Joback Method
cpg	646.49	J/mol×K	811.00	Joback Method
cpg	659.41	J/mol×K	845.75	Joback Method
cpg	671.52	J/mol×K	880.51	Joback Method
cpg	682.88	J/mol×K	915.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308648&Units=SI
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

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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