

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

Inchi: InChI=1S/C16H16BrNO/c1-3-18(15-9-4-6-12(2)10-15)16(19)13-7-5-8-14(17)11-13/h4-11

InchiKey: LRAJOVQWYFWYJH-UHFFFAOYSA-N

Formula: C16H16BrNO

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

Mol. weight [g/mol]: 318.21

Physical Properties

Property code	Value	Unit	Source
gf	285.58	kJ/mol	Joback Method
hf	57.83	kJ/mol	Joback Method
hfus	34.40	kJ/mol	Joback Method
hvap	72.31	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	4.424		Crippen Method
mcvol	217.830	ml/mol	McGowan Method
pc	2520.12	kPa	Joback Method
rinpol	2027.00		NIST Webbook
rinpol	2027.00		NIST Webbook
tb	761.27	K	Joback Method
tc	1005.54	K	Joback Method
tf	490.16	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.67	J/mol×K	761.27	Joback Method
cpg	582.19	J/mol×K	801.98	Joback Method
cpg	595.52	J/mol×K	842.69	Joback Method
cpg	607.78	J/mol×K	883.41	Joback Method
cpg	619.05	J/mol×K	924.12	Joback Method
cpg	629.43	J/mol×K	964.83	Joback Method
cpg	639.04	J/mol×K	1005.54	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=U308621&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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