2-Bromo-2-ethylbutylamide

Inchi: InChI=1S/C6H12BrNO/c1-3-6(7,4-2)5(8)9/h3-4H2,1-2H3,(H2,8,9)
InchiKey: ACEYAMOAGUDVAQ-UHFFFAOYSA-N
Formula: C6H12BrNO
SMILES: CCC(Br)(CC)C(N)=O
Mol. weight [g/mol]: 194.07

Physical Properties

Property code	Value	Unit	Source
hf	-308.01	kJ/mol	Cheméo Relay (1.0)
hfus	15.96	kJ/mol	Joback Method
log10ws	-1.89		Cheméo Relay (1.0)
logp	1.425		Crippen Method
mcvol	124.450	ml/mol	McGowan Method
tb	498.59	K	Cheméo Relay (1.0)
tf	322.16	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.57	J/mol×K	526.01	Joback Method
cpg	278.58	J/mol×K	562.67	Joback Method
cpg	288.81	J/mol×K	599.34	Joback Method
cpg	298.32	J/mol×K	636.00	Joback Method
cpg	307.17	J/mol×K	672.66	Joback Method
cpg	315.39	J/mol×K	709.33	Joback Method
cpg	323.04	J/mol×K	745.99	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C511706
Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point