

Butanamide, N-(4-bromophenyl)-2,2,3,3,4,4,4-heptafluoro-

Inchi: InChI=1S/C10H5BrF7NO/c11-5-1-3-6(4-2-5)19-7(20)8(12,13)9(14,15)10(16,17)18/h1-4H

InchiKey: GZPNVRALAPIZMQ-UHFFFAOYSA-N

Formula: C10H5BrF7NO

SMILES: O=C(Nc1ccc(Br)cc1)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 368.05

Physical Properties

Property code	Value	Unit	Source
gf	-1244.26	kJ/mol	Joback Method
hf	-1456.47	kJ/mol	Joback Method
hfus	26.61	kJ/mol	Joback Method
hvap	50.80	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.221		Crippen Method
mcvol	169.440	ml/mol	McGowan Method
pc	2563.69	kPa	Joback Method
rinqol	1400.00		NIST Webbook
tb	615.26	K	Joback Method
tc	811.69	K	Joback Method
tf	415.18	K	Joback Method
vc	0.683	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.25	J/mol×K	615.26	Joback Method
cpg	438.18	J/mol×K	648.00	Joback Method
cpg	447.17	J/mol×K	680.74	Joback Method
cpg	455.29	J/mol×K	713.47	Joback Method
cpg	462.64	J/mol×K	746.21	Joback Method
cpg	469.30	J/mol×K	778.95	Joback Method
cpg	475.35	J/mol×K	811.69	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=U307279&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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