

2,5-Difluorobenzamide, N-(4-bromophenyl)-

Inchi:	InChI=1S/C13H8BrF2NO/c14-8-1-4-10(5-2-8)17-13(18)11-7-9(15)3-6-12(11)16/h1-7H,(H
InchiKey:	JVFSVFOJFVHTHF-UHFFFAOYSA-N
Formula:	C13H8BrF2NO
SMILES:	O=C(Nc1ccc(Br)cc1)c1cc(F)ccc1F
Mol. weight [g/mol]:	312.11

Physical Properties

Property code	Value	Unit	Source
gf	-160.32	kJ/mol	Joback Method
hf	-298.00	kJ/mol	Joback Method
hfus	34.48	kJ/mol	Joback Method
hvap	69.05	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	3.980		Crippen Method
mcvol	179.100	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
rinpol	2211.00		NIST Webbook
rinpol	2211.00		NIST Webbook
tb	733.88	K	Joback Method
tc	973.31	K	Joback Method
tf	490.24	K	Joback Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.99	J/molxK	733.88	Joback Method
cpg	446.89	J/molxK	773.78	Joback Method
cpg	456.86	J/molxK	813.69	Joback Method
cpg	465.96	J/molxK	853.59	Joback Method
cpg	474.26	J/molxK	893.50	Joback Method
cpg	481.82	J/molxK	933.40	Joback Method
cpg	488.70	J/molxK	973.31	Joback Method

Sources

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=U358050&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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