Benzamide, N-(4-bromophenyl)-2,6-difluoro-

Inchi: InChI=1S/C13H8BrF2NO/c14-8-4-6-9(7-5-8)17-13(18)12-10(15)2-1-3-11(12)16/h1-7H,(H
InchiKey: LVUNQOIPWNMCLV-UHFFFAOYSA-N
Formula: C13H8BrF2NO
SMILES: O=C(Nc1ccc(Br)cc1)c1c(F)cccc1F
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	2173.00		NIST Webbook
rinpol	2173.00		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/mol×K	733.88	Joback Method
cpg	446.89	J/mol×K	773.78	Joback Method
cpg	456.86	J/mol×K	813.69	Joback Method
cpg	465.96	J/mol×K	853.59	Joback Method
cpg	474.26	J/mol×K	893.50	Joback Method
cpg	481.82	J/mol×K	933.40	Joback Method
cpg	488.70	J/mol×K	973.31	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=U307431&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume