Benzamide, N-(2-iodo-4-methylphenyl)-3-trifluoromethyl-

Inchi: InChI=1S/C15H11F3INO/c1-9-5-6-13(12(19)7-9)20-14(21)10-3-2-4-11(8-10)15(16,17)18/

InchiKey: GJCZZIMCPGAIDE-UHFFFAOYSA-N

Formula: C15H11F3INO

SMILES: Cc1ccc(NC(=O)c2cccc(C(F)(F)F)c2)c(I)c1

Mol. weight [g/mol]: 405.15

Physical Properties

Property code	Value	Unit	Source
gf	-291.65	kJ/mol	Joback Method
hf	-493.60	kJ/mol	Joback Method
hfus	34.45	kJ/mol	Joback Method
hvap	74.33	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	4.871		Crippen Method
mcvol	217.370	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
rinpol	2355.00		NIST Webbook
tb	802.66	K	Joback Method
tc	1047.73	K	Joback Method
tf	514.05	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.70	J/mol×K	802.66	Joback Method
cpg	569.91	J/mol×K	843.51	Joback Method
cpg	580.14	J/mol×K	884.35	Joback Method
cpg	589.51	J/mol×K	925.20	Joback Method
cpg	598.12	J/mol×K	966.04	Joback Method
cpg	606.08	J/mol×K	1006.89	Joback Method
cpg	613.52	J/mol×K	1047.73	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=U306941&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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