Acetamide, N-(2-iodo-4-methylphenyl)-2,2,2-trifluoro-

Inchi: InChI=1S/C9H7F3INO/c1-5-2-3-7(6(13)4-5)14-8(15)9(10,11)12/h2-4H,1H3,(H,14,15)
InchiKey: DZNFDYLOBOIWCO-UHFFFAOYSA-N
Formula: C9H7F3INO
SMILES: Cc1ccc(NC(=O)C(F)(F)F)c(I)c1
Mol. weight [g/mol]: 329.06

Physical Properties

Property code	Value	Unit	Source
gf	-444.95	kJ/mol	Joback Method
hf	-594.82	kJ/mol	Joback Method
hfus	25.26	kJ/mol	Joback Method
hvap	58.04	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.100		Crippen Method
mcvol	156.590	ml/mol	McGowan Method
pc	2944.08	kPa	Joback Method
rinpol	1518.00		NIST Webbook
tb	633.72	K	Joback Method
tc	862.60	K	Joback Method
tf	407.49	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.42	J/mol×K	633.72	Joback Method
cpg	359.32	J/mol×K	671.87	Joback Method
cpg	368.38	J/mol×K	710.01	Joback Method
cpg	376.66	J/mol×K	748.16	Joback Method
cpg	384.24	J/mol×K	786.30	Joback Method
cpg	391.18	J/mol×K	824.45	Joback Method
cpg	397.55	J/mol×K	862.60	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U307315&Units=SI

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