Propanamide, N-(2-iodo-4-methylphenyl)-2,2,3,3,3-pentafluoro-

Inchi: InChI=1S/C10H7F5INO/c1-5-2-3-7(6(16)4-5)17-8(18)9(11,12)10(13,14)15/h2-4H,1H3,(H

InchiKey: MHDRBTLQQFRCLE-UHFFFAOYSA-N

Formula: C10H7F5INO

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

Mol. weight [g/mol]: 379.07

Physical Properties

Property code	Value	Unit	Source
gf	-823.31	kJ/mol	Joback Method
hf	-1016.43	kJ/mol	Joback Method
hfus	26.60	kJ/mol	Joback Method
hvap	57.33	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	3.736		Crippen Method
mcvol	174.220	ml/mol	McGowan Method
pc	2475.19	kPa	Joback Method
rinpol	1521.00		NIST Webbook
tb	651.91	K	Joback Method
tc	868.75	K	Joback Method
tf	422.36	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.62	J/mol×K	651.91	Joback Method
cpg	426.55	J/mol×K	688.05	Joback Method
cpg	435.58	J/mol×K	724.19	Joback Method
cpg	443.81	J/mol×K	760.33	Joback Method
cpg	451.31	J/mol×K	796.47	Joback Method
cpg	458.17	J/mol×K	832.61	Joback Method
cpg	464.47	J/mol×K	868.75	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=U307336&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

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