Butanamide, N-(2-iodo-4-methylphenyl)-2,2,3,3,4,4,4-heptafluor

Inchi: InChI=1S/C11H7F7INO/c1-5-2-3-7(6(19)4-5)20-8(21)9(12,13)10(14,15)11(16,17)18/h2-4

InchiKey: AQAMNUJMQDJRFI-UHFFFAOYSA-N

Formula: C11H7F7INO

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

Mol. weight [g/mol]: 429.07

Physical Properties

Property code	Value	Unit	Source
gf	-1201.67	kJ/mol	Joback Method
hf	-1438.04	kJ/mol	Joback Method
hfus	27.93	kJ/mol	Joback Method
hvap	56.63	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.371		Crippen Method
mcvol	191.850	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
rinpol	1556.00		NIST Webbook
tb	670.10	K	Joback Method
tc	876.57	K	Joback Method
tf	437.23	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.59	J/mol×K	670.10	Joback Method
cpg	494.42	J/mol×K	704.51	Joback Method
cpg	503.33	J/mol×K	738.92	Joback Method
cpg	511.43	J/mol×K	773.34	Joback Method
cpg	518.81	J/mol×K	807.75	Joback Method
cpg	525.56	J/mol×K	842.16	Joback Method
cpg	531.78	J/mol×K	876.57	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=U307282&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