Benzamide, N-(2-iodo-4-methylphenyl)-4-butyl-

Inchi: InChI=1S/C18H20INO/c1-3-4-5-14-7-9-15(10-8-14)18(21)20-17-11-6-13(2)12-16(17)19/h
InchiKey: NWJUWXIVNGCVLN-UHFFFAOYSA-N
Formula: C18H20INO
SMILES: CCCCc1ccc(C(=O)Nc2ccc(C)cc2I)cc1
Mol. weight [g/mol]: 393.26

Physical Properties

Property code	Value	Unit	Source
gf	315.20	kJ/mol	Joback Method
hf	41.56	kJ/mol	Joback Method
hfus	40.39	kJ/mol	Joback Method
hvap	84.75	kJ/mol	Joback Method
log10ws	-6.71		Crippen Method
logp	5.195		Crippen Method
mcvol	254.330	ml/mol	McGowan Method
pc	1932.13	kPa	Joback Method
rinpol	2931.00		NIST Webbook
rinpol	2931.00		NIST Webbook
tb	876.72	K	Joback Method
tc	1125.42	K	Joback Method
tf	543.67	K	Joback Method
vc	0.957	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.04	J/mol×K	876.72	Joback Method
cpg	712.81	J/mol×K	918.17	Joback Method
cpg	725.49	J/mol×K	959.62	Joback Method
cpg	737.16	J/mol×K	1001.07	Joback Method
cpg	747.92	J/mol×K	1042.52	Joback Method
cpg	757.86	J/mol×K	1083.97	Joback Method
cpg	767.08	J/mol×K	1125.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306997&Units=SI
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

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