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

Inchi: InChI=1S/C16H16INO/c1-3-12-5-7-13(8-6-12)16(19)18-15-9-4-11(2)10-14(15)17/h4-10H
InchiKey: SAKWCZALYGHLBO-UHFFFAOYSA-N
Formula: C16H16INO
SMILES: CCc1ccc(C(=O)Nc2ccc(C)cc2I)cc1
Mol. weight [g/mol]: 365.21

Physical Properties

Property code	Value	Unit	Source
gf	298.36	kJ/mol	Joback Method
hf	82.84	kJ/mol	Joback Method
hfus	35.21	kJ/mol	Joback Method
hvap	80.30	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	4.414		Crippen Method
mcvol	226.150	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
rinpol	2687.00		NIST Webbook
tb	830.96	K	Joback Method
tc	1089.23	K	Joback Method
tf	521.13	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	587.84	J/mol×K	830.96	Joback Method
cpg	601.07	J/mol×K	874.00	Joback Method
cpg	613.18	J/mol×K	917.05	Joback Method
cpg	624.26	J/mol×K	960.09	Joback Method
cpg	634.40	J/mol×K	1003.14	Joback Method
cpg	643.70	J/mol×K	1046.18	Joback Method
cpg	652.26	J/mol×K	1089.23	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=U307020&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