Benzalhippuric acid

Inchi: InChI=1S/C16H13NO3/c18-15(13-9-5-2-6-10-13)17-14(16(19)20)11-12-7-3-1-4-8-12/h1-1
InchiKey: HHWCUKQKFIVCEZ-SDNWHVSQSA-N
Formula: C16H13NO3
SMILES: O=C(O)C(=Cc1ccccc1)NC(=O)c1ccccc1
Mol. weight [g/mol]: 267.28
CAS: 1155-48-2

Physical Properties

Property code	Value	Unit	Source
chs	-7769.40	kJ/mol	NIST Webbook
gf	75.06	kJ/mol	Joback Method
hf	-117.00	kJ/mol	Joback Method
hfus	36.55	kJ/mol	Joback Method
hvap	92.41	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	2.542		Crippen Method
mcvol	203.470	ml/mol	McGowan Method
pc	3072.75	kPa	Joback Method
tb	872.97	K	Joback Method
tc	1106.87	K	Joback Method
tf	517.22	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.93	J/mol×K	872.97	Joback Method
cpg	590.17	J/mol×K	911.95	Joback Method
cpg	599.61	J/mol×K	950.94	Joback Method
cpg	608.33	J/mol×K	989.92	Joback Method
cpg	616.44	J/mol×K	1028.90	Joback Method
cpg	624.05	J/mol×K	1067.89	Joback Method
cpg	631.24	J/mol×K	1106.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1155482&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

Legend

chs:	Standard solid enthalpy of combustion
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume