8-Carboxynaphyhalene-1-carboxamide

Inchi: InChI=1S/C12H9NO3/c13-11(14)8-5-1-3-7-4-2-6-9(10(7)8)12(15)16/h1-6H,(H2,13,14)(H,
InchiKey: GRVIMBYDMARKEZ-UHFFFAOYSA-N
Formula: C12H9NO3
SMILES: NC(=O)c1cccc2cccc(C(=O)O)c12
Mol. weight [g/mol]: 215.20
CAS: 5811-88-1

Physical Properties

Property code	Value	Unit	Source
gf	-78.25	kJ/mol	Joback Method
hf	-229.95	kJ/mol	Joback Method
hfus	29.60	kJ/mol	Joback Method
hvap	88.36	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	1.637		Crippen Method
mcvol	155.710	ml/mol	McGowan Method
pc	4167.71	kPa	Joback Method
tb	802.03	K	Joback Method
tc	1033.38	K	Joback Method
tf	553.10	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.22	J/mol×K	802.03	Joback Method
cpg	426.71	J/mol×K	840.59	Joback Method
cpg	434.56	J/mol×K	879.15	Joback Method
cpg	441.83	J/mol×K	917.70	Joback Method
cpg	448.59	J/mol×K	956.26	Joback Method
cpg	454.89	J/mol×K	994.82	Joback Method
cpg	460.82	J/mol×K	1033.38	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=C5811881&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume