5-Phenyl-2,3,4,5-tetrahydrobenzoxepin-5-carboxa

Inchi: InChI=1S/C17H17NO2/c18-16(19)17(13-7-2-1-3-8-13)11-6-12-20-15-10-5-4-9-14(15)17/h
InchiKey: PKIZNLKQWLSCFP-UHFFFAOYSA-N
Formula: C17H17NO2
SMILES: NC(=O)C1(c2ccccc2)CCCOc2ccccc21
Mol. weight [g/mol]: 267.32
CAS: 94908-49-3

Physical Properties

Property code	Value	Unit	Source
gf	189.92	kJ/mol	Joback Method
hf	-67.69	kJ/mol	Joback Method
hfus	29.89	kJ/mol	Joback Method
hvap	79.65	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	2.631		Crippen Method
mcvol	209.430	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
tb	815.57	K	Joback Method
tc	1088.20	K	Joback Method
tf	541.27	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.17	J/mol×K	815.57	Joback Method
cpg	640.62	J/mol×K	861.01	Joback Method
cpg	657.44	J/mol×K	906.45	Joback Method
cpg	673.95	J/mol×K	951.89	Joback Method
cpg	690.44	J/mol×K	997.32	Joback Method
cpg	707.24	J/mol×K	1042.76	Joback Method
cpg	724.64	J/mol×K	1088.20	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94908493&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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