4-Benzyl-2,5-oxazolidinedione

Inchi: InChI=1S/C10H9NO3/c12-9-8(11-10(13)14-9)6-7-4-2-1-3-5-7/h1-5,8H,6H2,(H,11,13)
InchiKey: GQBIVYSGPXCELZ-UHFFFAOYSA-N
Formula: C10H9NO3
SMILES: O=C1OC(O)=NC1Cc1ccccc1
Mol. weight [g/mol]: 191.18
CAS: 1892-35-9

Physical Properties

Property code	Value	Unit	Source
chs	-4668.90 ± 3.30	kJ/mol	NIST Webbook
gf	-26.14	kJ/mol	Joback Method
hf	-257.37	kJ/mol	Joback Method
hfs	-552.40 ± 3.40	kJ/mol	NIST Webbook
hfus	27.18	kJ/mol	Joback Method
hvap	72.99	kJ/mol	Joback Method
log10ws	-1.46		Crippen Method
logp	1.068		Crippen Method
mcvol	136.130	ml/mol	McGowan Method
pc	4288.66	kPa	Joback Method
tb	714.95	K	Joback Method
tc	954.94	K	Joback Method
tf	480.21	K	Joback Method
vc	0.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.26	J/mol×K	714.95	Joback Method
cpg	403.98	J/mol×K	754.95	Joback Method
cpg	415.60	J/mol×K	794.95	Joback Method
cpg	426.12	J/mol×K	834.95	Joback Method
cpg	435.52	J/mol×K	874.94	Joback Method
cpg	443.80	J/mol×K	914.94	Joback Method
cpg	450.94	J/mol×K	954.94	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=C1892359&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hfs:	Solid phase 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

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