Dibenz[b,f]][1,4]oxazepine

Other names:	CR
	EA 3547
	Dibenzoxazepine
	Cr (lacrimator)
	Dibenz(b,f)-1,4-oxazepin
	dibenz-(b,f)-1,4-oxazephine
Inchi:	InChI=1S/C13H9NO/c1-3-7-12-10(5-1)9-14-11-6-2-4-8-13(11)15-12/h1-9H
InchiKey:	NPUACKRELIJTFM-UHFFFAOYSA-N
Formula:	C13H9NO
SMILES:	C1=Nc2ccccc2Oc2ccccc21
Mol. weight [g/mol]:	195.22
CAS:	257-07-8

Physical Properties

Property code	Value	Unit	Source
gf	393.22	kJ/mol	Joback Method
hf	228.36	kJ/mol	Joback Method
hfus	28.13	kJ/mol	Joback Method
hvap	61.64	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	3.543		Crippen Method
mcvol	147.200	ml/mol	McGowan Method
pc	3704.46	kPa	Joback Method
rinpol	1811.00		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1811.00		NIST Webbook
ripol	2813.00		NIST Webbook
ripol	2813.00		NIST Webbook
ripol	2813.40		NIST Webbook
ripol	2813.40		NIST Webbook
tb	651.38	K	Joback Method
tc	922.92	K	Joback Method
tf	435.20	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.12	J/mol×K	651.38	Joback Method
cpg	392.36	J/mol×K	696.64	Joback Method
cpg	406.16	J/mol×K	741.89	Joback Method
cpg	418.63	J/mol×K	787.15	Joback Method
cpg	429.87	J/mol×K	832.40	Joback Method
cpg	440.02	J/mol×K	877.66	Joback Method
cpg	449.17	J/mol×K	922.92	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=C257078&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume