Propallylonal M (des-Br, OH)

Inchi: InChI=1S/C10H16N2O4/c1-5(2)10(4-6(3)13)7(14)11-9(16)12-8(10)15/h5-6,13H,4H2,1-3H
InchiKey: PKMMAWVSVCNKLQ-UHFFFAOYSA-N
Formula: C10H16N2O4
SMILES: CC(O)CC1(C(C)C)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 228.25

Physical Properties

Property code	Value	Unit	Source
gf	-281.77	kJ/mol	Joback Method
hf	-680.44	kJ/mol	Joback Method
hfus	21.95	kJ/mol	Joback Method
hvap	79.29	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	-0.234		Crippen Method
mcvol	171.440	ml/mol	McGowan Method
pc	3607.21	kPa	Joback Method
rinpol	1770.00		NIST Webbook
rinpol	1770.00		NIST Webbook
tb	839.85	K	Joback Method
tc	1080.60	K	Joback Method
tf	679.28	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.59	J/mol×K	839.85	Joback Method
cpg	566.80	J/mol×K	879.98	Joback Method
cpg	581.16	J/mol×K	920.10	Joback Method
cpg	594.66	J/mol×K	960.23	Joback Method
cpg	607.33	J/mol×K	1000.35	Joback Method
cpg	619.16	J/mol×K	1040.48	Joback Method
cpg	630.16	J/mol×K	1080.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R57630&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume