[3.3.3]Propellane-2-one, 8-methylene

Inchi: InChI=1S/C12H16O/c1-9-3-7-11-5-2-6-12(9,11)10(13)4-8-11/h1-8H2
InchiKey: HAWQSAGPCXMKQJ-UHFFFAOYSA-N
Formula: C12H16O
SMILES: C=C1CCC23CCCC12C(=O)CC3
Mol. weight [g/mol]: 176.25
CAS: 112138-33-7

Physical Properties

Property code	Value	Unit	Source
gf	135.43	kJ/mol	Joback Method
hf	-87.57	kJ/mol	Joback Method
hfus	1.73	kJ/mol	Joback Method
hvap	44.80	kJ/mol	Joback Method
ie	8.90	eV	NIST Webbook
log10ws	-3.18		Crippen Method
logp	2.856		Crippen Method
mcvol	144.630	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
tb	574.85	K	Joback Method
tc	828.03	K	Joback Method
tf	405.72	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.24	J/mol×K	574.85	Joback Method
cpg	403.17	J/mol×K	617.05	Joback Method
cpg	420.66	J/mol×K	659.24	Joback Method
cpg	437.10	J/mol×K	701.44	Joback Method
cpg	452.86	J/mol×K	743.64	Joback Method
cpg	468.33	J/mol×K	785.84	Joback Method
cpg	483.91	J/mol×K	828.03	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112138337&Units=SI

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
ie:	Ionization energy
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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