«gamma»-Campholenal

Inchi: InChI=1S/C10H18O/c1-8-4-5-9(6-7-11)10(8,2)3/h9,11H,1,4-7H2,2-3H3
InchiKey: WBHCKTOVJQYUQV-UHFFFAOYSA-N
Formula: C10H18O
SMILES: C=C1CCC(CCO)C1(C)C
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
gf	-27.07	kJ/mol	Joback Method
hf	-262.34	kJ/mol	Joback Method
hfus	13.29	kJ/mol	Joback Method
hvap	53.49	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.361		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
rinpol	1067.00		NIST Webbook
rinpol	1067.00		NIST Webbook
ripol	1435.00		NIST Webbook
ripol	1435.00		NIST Webbook
tb	530.39	K	Joback Method
tc	718.51	K	Joback Method
tf	307.52	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.45	J/mol×K	530.39	Joback Method
cpg	363.96	J/mol×K	561.74	Joback Method
cpg	377.69	J/mol×K	593.10	Joback Method
cpg	390.73	J/mol×K	624.45	Joback Method
cpg	403.14	J/mol×K	655.80	Joback Method
cpg	415.01	J/mol×K	687.16	Joback Method

cpg	426.39	J/mol×K	718.51	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=R204649&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
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