(6R,7aS)-3,6-Dimethyl-5,6,7,7a-tetrahydrobenzofu

Inchi: InChI=1S/C10H14O2/c1-6-3-4-8-7(2)10(11)12-9(8)5-6/h6,9H,3-5H2,1-2H3
InchiKey: VUVQBYIJRDUVHT-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: CC1=C2CCC(C)CC2OC1=O
Mol. weight [g/mol]: 166.22
CAS: 75684-66-1

Physical Properties

Property code	Value	Unit	Source
gf	-79.49	kJ/mol	Joback Method
hf	-357.47	kJ/mol	Joback Method
hfus	19.56	kJ/mol	Joback Method
hvap	48.57	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.048		Crippen Method
mcvol	133.180	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
rinpol	1531.10		NIST Webbook
rinpol	1531.10		NIST Webbook
ripol	2422.00		NIST Webbook
ripol	2422.00		NIST Webbook
tb	558.38	K	Joback Method
tc	791.07	K	Joback Method
tf	348.37	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.43	J/mol×K	558.38	Joback Method
cpg	355.83	J/mol×K	597.16	Joback Method
cpg	372.24	J/mol×K	635.94	Joback Method
cpg	387.67	J/mol×K	674.73	Joback Method
cpg	402.16	J/mol×K	713.51	Joback Method

cpg	415.71	J/mol×K	752.29	Joback Method
cpg	428.34	J/mol×K	791.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75684661&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

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

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