Exo-2-methyl-7-oxabi-cyclo[2.2.1]heptane

Inchi: InChI=1S/C7H12O/c1-5-4-6-2-3-7(5)8-6/h5-7H,2-4H2,1H3/t5-,6?,7?/m1/s1
InchiKey: YSPMLGNTRGMJLE-GRQBKTHUSA-N
Formula: C7H12O
SMILES: CC1CC2CCC1O2
Mol. weight [g/mol]: 112.17
CAS: 16325-23-8

Physical Properties

Property code	Value	Unit	Source
chl	-4215.70 ± 1.70	kJ/mol	NIST Webbook
chl	-4215.70 ± 1.70	kJ/mol	NIST Webbook
gf	23.63	kJ/mol	Joback Method
hf	-200.71	kJ/mol	Joback Method
hfl	-253.80 ± 2.20	kJ/mol	NIST Webbook
hfus	17.11	kJ/mol	Joback Method
hvap	35.38	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	1.574		Crippen Method
mcvol	93.640	ml/mol	McGowan Method
pc	3686.49	kPa	Joback Method
tb	399.59	K	Joback Method
tc	602.57	K	Joback Method
tf	223.34	K	Joback Method
vc	0.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.57	J/mol×K	399.59	Joback Method
cpg	260.98	J/mol×K	568.74	Joback Method
cpg	248.61	J/mol×K	534.91	Joback Method
cpg	235.44	J/mol×K	501.08	Joback Method
cpg	221.40	J/mol×K	467.25	Joback Method
cpg	206.46	J/mol×K	433.42	Joback Method

cpg	272.58	J/mol×K	602.57	Joback Method
dvisc	0.0005708	Pa×s	399.59	Joback Method
dvisc	0.0005857	Pa×s	370.21	Joback Method
dvisc	0.0006038	Pa×s	340.84	Joback Method
dvisc	0.0006260	Pa×s	311.46	Joback Method
dvisc	0.0006539	Pa×s	282.09	Joback Method
dvisc	0.0006900	Pa×s	252.72	Joback Method
dvisc	0.0007384	Pa×s	223.34	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=C16325238&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume