endo-2-Norborneol acetate

Inchi: InChI=1S/C9H14O2/c1-6(10)11-9-5-7-2-3-8(9)4-7/h7-9H,2-5H2,1H3/t7?,8?,9-/m0/s1
InchiKey: YXNICIBZSREEPY-AMDVSUOASA-N
Formula: C9H14O2
SMILES: CC(=O)O[C@H]1CC2CCC1C2
Mol. weight [g/mol]: 154.21

Physical Properties

Property code	Value	Unit	Source
hf	-477.52	kJ/mol	Cheméo Relay (1.0)
hfus	17.09	kJ/mol	Joback Method
ie	9.54	eV	Cheméo Relay (1.0)
logp	1.738		Crippen Method
mcvol	123.390	ml/mol	McGowan Method
rinpol	1111.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1125.00		NIST Webbook
tb	465.43	K	Cheméo Relay (1.0)
tf	266.47	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.85	J/mol×K	494.69	Joback Method
cpg	311.49	J/mol×K	529.48	Joback Method
cpg	327.15	J/mol×K	564.28	Joback Method
cpg	341.89	J/mol×K	599.07	Joback Method
cpg	355.75	J/mol×K	633.86	Joback Method
cpg	368.76	J/mol×K	668.65	Joback Method
cpg	380.99	J/mol×K	703.45	Joback Method
dvisc	0.0015354	Pa×s	291.47	Joback Method
dvisc	0.0013027	Pa×s	325.34	Joback Method
dvisc	0.0011401	Pa×s	359.21	Joback Method
dvisc	0.0010209	Pa×s	393.08	Joback Method
dvisc	0.0009304	Pa×s	426.95	Joback Method

dvisc	0.0008595	Pa×s	460.82	Joback Method
dvisc	0.0008027	Pa×s	494.69	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R239031&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

ie: Ionization energy

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point