7-Oxabicyclo[4.1.0]heptane-3-carboxylic acid, 4-methyl-, 4-methyl-7-oxabicyclo-[4.1.0]heptyl methyl ester

Inchi: InChI=1S/C16H24O4/c1-8-3-12-14(19-12)5-10(8)7-18-16(17)11-6-15-13(20-15)4-9(11)2/
InchiKey: GRWFFFOEIHGUBG-UHFFFAOYSA-N
Formula: C16H24O4
SMILES: CC1CC2OC2CC1COC(=O)C1CC2OC2CC1C
Mol. weight [g/mol]: 280.36
CAS: 141-37-7

Physical Properties

Property code	Value	Unit	Source
gf	-134.36	kJ/mol	Joback Method
hf	-684.85	kJ/mol	Joback Method
hfus	48.56	kJ/mol	Joback Method
hvap	68.15	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.157		Crippen Method
mcvol	212.040	ml/mol	McGowan Method
pc	1910.24	kPa	Joback Method
tb	712.49	K	Joback Method
tc	929.05	K	Joback Method
tf	443.14	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.04	J/mol×K	712.49	Joback Method
cpg	726.23	J/mol×K	748.58	Joback Method
cpg	746.04	J/mol×K	784.68	Joback Method
cpg	764.56	J/mol×K	820.77	Joback Method
cpg	781.87	J/mol×K	856.87	Joback Method
cpg	798.08	J/mol×K	892.96	Joback Method
cpg	813.26	J/mol×K	929.05	Joback Method
dvisc	0.0067202	Pa×s	443.14	Joback Method
dvisc	0.0067039	Pa×s	488.03	Joback Method

dvisc	0.0066905	Pa×s	532.92	Joback Method
dvisc	0.0066791	Pa×s	577.82	Joback Method
dvisc	0.0066694	Pa×s	622.71	Joback Method
dvisc	0.0066611	Pa×s	667.60	Joback Method
dvisc	0.0066538	Pa×s	712.49	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C141377&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

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

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume