Bicyclo[2.2.1]hept-5-ene-2,3-dicarboxylic acid, diethyl ester

Other names: Diethyl bicyclo[2.2.1]hept-5-ene-2,3-dicarboxylate
Inchi: InChI=1S/C13H18O4/c1-3-16-12(14)10-8-5-6-9(7-8)11(10)13(15)17-4-2/h5-6,8-11H,3-4,7
InchiKey: UXRMRBNLTQHPEU-UHFFFAOYSA-N
Formula: C13H18O4
SMILES: CCOC(=O)C1C2C=CC(C2)C1C(=O)OCC
Mol. weight [g/mol]: 238.28
CAS: 5883-33-0

Physical Properties

Property code	Value	Unit	Source
gf	-285.32	kJ/mol	Joback Method
hf	-644.71	kJ/mol	Joback Method
hfus	32.53	kJ/mol	Joback Method
hvap	62.52	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	1.551		Crippen Method
mcvol	182.890	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
rinpol	1561.00		NIST Webbook
rinpol	1561.00		NIST Webbook
tb	656.99	K	Joback Method
tc	860.92	K	Joback Method
tf	405.23	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.03	J/mol×K	656.99	Joback Method
cpg	539.48	J/mol×K	690.98	Joback Method
cpg	554.96	J/mol×K	724.97	Joback Method
cpg	569.49	J/mol×K	758.96	Joback Method
cpg	583.12	J/mol×K	792.95	Joback Method
cpg	595.87	J/mol×K	826.94	Joback Method

cpg	607.77	J/mol×K	860.92	Joback Method
dvisc	0.0022244	Pa×s	405.23	Joback Method
dvisc	0.0018221	Pa×s	447.19	Joback Method
dvisc	0.0015445	Pa×s	489.15	Joback Method
dvisc	0.0013438	Pa×s	531.11	Joback Method
dvisc	0.0011933	Pa×s	573.07	Joback Method
dvisc	0.0010770	Pa×s	615.03	Joback Method
dvisc	0.0009848	Pa×s	656.99	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5883330&Units=SI

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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