Pentanoic acid, 2-methyl-, anhydride

Inchi: InChI=1S/C12H22O3/c1-5-7-9(3)11(13)15-12(14)10(4)8-6-2/h9-10H,5-8H2,1-4H3
InchiKey: NCYCWNILADFMPI-UHFFFAOYSA-N
Formula: C12H22O3
SMILES: CCCC(C)C(=O)OC(=O)C(C)CCC
Mol. weight [g/mol]: 214.30
CAS: 63169-61-9

Physical Properties

Property code	Value	Unit	Source
gf	-317.56	kJ/mol	Joback Method
hf	-658.95	kJ/mol	Joback Method
hfus	24.18	kJ/mol	Joback Method
hvap	57.43	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.929		Crippen Method
mcvol	188.950	ml/mol	McGowan Method
pc	1984.12	kPa	Joback Method
rinpol	1347.50		NIST Webbook
tb	603.24	K	Joback Method
tc	787.29	K	Joback Method
tf	317.09	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.53	J/mol×K	603.24	Joback Method
cpg	504.88	J/mol×K	633.91	Joback Method
cpg	519.51	J/mol×K	664.59	Joback Method
cpg	533.45	J/mol×K	695.26	Joback Method
cpg	546.69	J/mol×K	725.94	Joback Method
cpg	559.26	J/mol×K	756.61	Joback Method
cpg	571.15	J/mol×K	787.29	Joback Method
dvisc	0.0040877	Pa×s	317.09	Joback Method

dvisc	0.0016982	Pa×s	364.78	Joback Method
dvisc	0.0008644	Pa×s	412.47	Joback Method
dvisc	0.0005061	Pa×s	460.17	Joback Method
dvisc	0.0003276	Pa×s	507.86	Joback Method
dvisc	0.0002286	Pa×s	555.55	Joback Method
dvisc	0.0001688	Pa×s	603.24	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=C63169619&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