Adipic acid, butyl 3-oxobut-2-yl ester

Inchi: InChI=1S/C14H24O5/c1-4-5-10-18-13(16)8-6-7-9-14(17)19-12(3)11(2)15/h12H,4-10H2,1
InchiKey: VSRDRFACHKTMJU-UHFFFAOYSA-N
Formula: C14H24O5
SMILES: CCCCOC(=O)CCCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 272.34

Physical Properties

Property code	Value	Unit	Source
gf	-532.20	kJ/mol	Joback Method
hf	-939.75	kJ/mol	Joback Method
hfus	35.67	kJ/mol	Joback Method
hvap	71.43	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.411		Crippen Method
mcvol	224.570	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
rinpol	1802.00		NIST Webbook
tb	725.73	K	Joback Method
tc	911.61	K	Joback Method
tf	426.79	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.31	J/mol×K	725.73	Joback Method
cpg	658.97	J/mol×K	756.71	Joback Method
cpg	672.82	J/mol×K	787.69	Joback Method
cpg	685.86	J/mol×K	818.67	Joback Method
cpg	698.10	J/mol×K	849.65	Joback Method
cpg	709.54	J/mol×K	880.63	Joback Method
cpg	720.18	J/mol×K	911.61	Joback Method
dvisc	0.0013982	Pa×s	426.79	Joback Method
dvisc	0.0007307	Pa×s	476.61	Joback Method

dvisc	0.0004318	Pa×s	526.44	Joback Method
dvisc	0.0002795	Pa×s	576.26	Joback Method
dvisc	0.0001938	Pa×s	626.08	Joback Method
dvisc	0.0001419	Pa×s	675.91	Joback Method
dvisc	0.0001084	Pa×s	725.73	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=U353748&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