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

Inchi: InChI=1S/C16H28O5/c1-12(2)8-7-11-20-15(18)9-5-6-10-16(19)21-14(4)13(3)17/h12,14H
InchiKey: KBIOMBDNDXGHLQ-UHFFFAOYSA-N
Formula: C16H28O5
SMILES: CC(=O)C(C)OC(=O)CCCCC(=O)OCCCC(C)C
Mol. weight [g/mol]: 300.39

Physical Properties

Property code	Value	Unit	Source
gf	-517.80	kJ/mol	Joback Method
hf	-986.31	kJ/mol	Joback Method
hfus	37.32	kJ/mol	Joback Method
hvap	75.49	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.047		Crippen Method
mcvol	252.750	ml/mol	McGowan Method
pc	1498.83	kPa	Joback Method
rinpol	2004.00		NIST Webbook
rinpol	2004.00		NIST Webbook
tb	771.05	K	Joback Method
tc	959.08	K	Joback Method
tf	434.33	K	Joback Method
vc	0.974	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	757.14	J/mol×K	771.05	Joback Method
cpg	772.74	J/mol×K	802.39	Joback Method
cpg	787.40	J/mol×K	833.73	Joback Method
cpg	801.14	J/mol×K	865.07	Joback Method
cpg	813.97	J/mol×K	896.40	Joback Method
cpg	825.88	J/mol×K	927.74	Joback Method
cpg	836.89	J/mol×K	959.08	Joback Method
dvisc	0.0013691	Pa×s	434.33	Joback Method

dvisc	0.0006419	Pa×s	490.45	Joback Method
dvisc	0.0003516	Pa×s	546.57	Joback Method
dvisc	0.0002154	Pa×s	602.69	Joback Method
dvisc	0.0001435	Pa×s	658.81	Joback Method
dvisc	0.0001019	Pa×s	714.93	Joback Method
dvisc	0.0000760	Pa×s	771.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353749&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

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