Adipic acid, isobutyl 4-methylpent-2-yl ester

Inchi: InChI=1S/C16H30O4/c1-12(2)10-14(5)20-16(18)9-7-6-8-15(17)19-11-13(3)4/h12-14H,6-1
InchiKey: GMVPLWJHPXIVGS-UHFFFAOYSA-N
Formula: C16H30O4
SMILES: CC(C)COC(=O)CCCCC(=O)OC(C)CC(C)C
Mol. weight [g/mol]: 286.41

Physical Properties

Property code	Value	Unit	Source
gf	-391.32	kJ/mol	Joback Method
hf	-879.01	kJ/mol	Joback Method
hfus	32.20	kJ/mol	Joback Method
hvap	68.36	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.724		Crippen Method
mcvol	251.180	ml/mol	McGowan Method
pc	1436.98	kPa	Joback Method
rinpol	1779.00		NIST Webbook
rinpol	1779.00		NIST Webbook
tb	716.74	K	Joback Method
tc	899.00	K	Joback Method
tf	369.40	K	Joback Method
vc	0.962	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.04	J/mol×K	716.74	Joback Method
cpg	812.14	J/mol×K	868.62	Joback Method
cpg	798.48	J/mol×K	838.25	Joback Method
cpg	783.94	J/mol×K	807.87	Joback Method
cpg	768.53	J/mol×K	777.49	Joback Method
cpg	752.23	J/mol×K	747.12	Joback Method
cpg	824.95	J/mol×K	899.00	Joback Method
dvisc	0.0000731	Pa×s	716.74	Joback Method

dvisc	0.0001014	Pa×s	658.85	Joback Method
dvisc	0.0001497	Pa×s	600.96	Joback Method
dvisc	0.0002403	Pa×s	543.07	Joback Method
dvisc	0.0004318	Pa×s	485.18	Joback Method
dvisc	0.0009093	Pa×s	427.29	Joback Method
dvisc	0.0024183	Pa×s	369.40	Joback Method

Sources

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=U353501&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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