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

Inchi: InChI=1S/C18H34O4/c1-5-6-7-10-13-21-17(19)11-8-9-12-18(20)22-16(4)14-15(2)3/h15-1
InchiKey: XBWPAQNRDBZFMI-UHFFFAOYSA-N
Formula: C18H34O4
SMILES: CCCCCCOC(=O)CCCCC(=O)OC(C)CC(C)C
Mol. weight [g/mol]: 314.46

Physical Properties

Property code	Value	Unit	Source
gf	-372.04	kJ/mol	Joback Method
hf	-915.01	kJ/mol	Joback Method
hfus	40.90	kJ/mol	Joback Method
hvap	73.20	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.648		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1241.58	kPa	Joback Method
rinpol	2011.00		NIST Webbook
rinpol	2011.00		NIST Webbook
tb	762.94	K	Joback Method
tc	944.42	K	Joback Method
tf	406.94	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.46	J/mol×K	762.94	Joback Method
cpg	929.48	J/mol×K	914.17	Joback Method
cpg	915.55	J/mol×K	883.93	Joback Method
cpg	900.70	J/mol×K	853.68	Joback Method
cpg	884.91	J/mol×K	823.43	Joback Method
cpg	868.17	J/mol×K	793.19	Joback Method
cpg	942.50	J/mol×K	944.42	Joback Method
dvisc	0.0000599	Pa×s	762.94	Joback Method

dvisc	0.0000818	Pa×s	703.61	Joback Method
dvisc	0.0001183	Pa×s	644.27	Joback Method
dvisc	0.0001844	Pa×s	584.94	Joback Method
dvisc	0.0003176	Pa×s	525.61	Joback Method
dvisc	0.0006283	Pa×s	466.27	Joback Method
dvisc	0.0015163	Pa×s	406.94	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=U353505&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