Adipic acid, 2,4-dimethylpent-3-yl pentyl ester

Inchi: InChI=1S/C18H34O4/c1-6-7-10-13-21-16(19)11-8-9-12-17(20)22-18(14(2)3)15(4)5/h14-1
InchiKey: MAFBFTLNTFTGDB-UHFFFAOYSA-N
Formula: C18H34O4
SMILES: CCCCCOC(=O)CCCCC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]: 314.46

Physical Properties

Property code	Value	Unit	Source
gf	-374.48	kJ/mol	Joback Method
hf	-920.29	kJ/mol	Joback Method
hfus	37.38	kJ/mol	Joback Method
hvap	72.81	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.504		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1248.61	kPa	Joback Method
rinpol	2000.00		NIST Webbook
rinpol	2000.00		NIST Webbook
tb	762.50	K	Joback Method
tc	945.56	K	Joback Method
tf	391.94	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.95	J/mol×K	762.50	Joback Method
cpg	868.82	J/mol×K	793.01	Joback Method
cpg	885.70	J/mol×K	823.52	Joback Method
cpg	901.60	J/mol×K	854.03	Joback Method
cpg	916.55	J/mol×K	884.54	Joback Method
cpg	930.54	J/mol×K	915.05	Joback Method
cpg	943.60	J/mol×K	945.56	Joback Method
dvisc	0.0019037	Pa×s	391.94	Joback Method

dvisc	0.0007062	Pa×s	453.70	Joback Method
dvisc	0.0003322	Pa×s	515.46	Joback Method
dvisc	0.0001837	Pa×s	577.22	Joback Method
dvisc	0.0001139	Pa×s	638.98	Joback Method
dvisc	0.0000768	Pa×s	700.74	Joback Method
dvisc	0.0000552	Pa×s	762.50	Joback Method

Sources

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=U349778&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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