Adipic acid, di(2,4-dimethylpent-3-yl) ester

Inchi: InChI=1S/C20H38O4/c1-13(2)19(14(3)4)23-17(21)11-9-10-12-18(22)24-20(15(5)6)16(7)8
InchiKey: ATADCGPMGKCFGA-UHFFFAOYSA-N
Formula: C20H38O4
SMILES: CC(C)C(OC(=O)CCCCC(=O)OC(C(C)C)C(C)C)C(C)C
Mol. weight [g/mol]: 342.51

Physical Properties

Property code	Value	Unit	Source
gf	-364.96	kJ/mol	Joback Method
hf	-977.41	kJ/mol	Joback Method
hfus	31.99	kJ/mol	Joback Method
hvap	76.10	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	4.994		Crippen Method
mcvol	307.540	ml/mol	McGowan Method
pc	1112.59	kPa	Joback Method
rinpol	2057.00		NIST Webbook
rinpol	2057.00		NIST Webbook
tb	806.94	K	Joback Method
tc	996.97	K	Joback Method
tf	369.48	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	972.05	J/mol×K	806.94	Joback Method
cpg	990.94	J/mol×K	838.61	Joback Method
cpg	1008.65	J/mol×K	870.28	Joback Method
cpg	1025.22	J/mol×K	901.95	Joback Method
cpg	1040.65	J/mol×K	933.63	Joback Method
cpg	1054.98	J/mol×K	965.30	Joback Method
cpg	1068.20	J/mol×K	996.97	Joback Method
dvisc	0.0032833	Pa×s	369.48	Joback Method

dvisc	0.0008030	Pa×s	442.39	Joback Method
dvisc	0.0002925	Pa×s	515.30	Joback Method
dvisc	0.0001369	Pa×s	588.21	Joback Method
dvisc	0.0000757	Pa×s	661.12	Joback Method
dvisc	0.0000471	Pa×s	734.03	Joback Method
dvisc	0.0000320	Pa×s	806.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353537&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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