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

Inchi: InChI=1S/C19H36O4/c1-14(2)10-9-13-22-17(20)11-7-8-12-18(21)23-19(15(3)4)16(5)6/h1
InchiKey: ADFPEMFGGNNRPA-UHFFFAOYSA-N
Formula: C19H36O4
SMILES: CC(C)CCCOC(=O)CCCCC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]: 328.49

Physical Properties

Property code	Value	Unit	Source
gf	-368.50	kJ/mol	Joback Method
hf	-946.21	kJ/mol	Joback Method
hfus	36.45	kJ/mol	Joback Method
hvap	74.65	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.750		Crippen Method
mcvol	293.450	ml/mol	McGowan Method
pc	1174.44	kPa	Joback Method
rinpol	2069.00		NIST Webbook
rinpol	2069.00		NIST Webbook
tb	784.94	K	Joback Method
tc	970.70	K	Joback Method
tf	388.21	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.84	J/mol×K	784.94	Joback Method
cpg	992.02	J/mol×K	939.74	Joback Method
cpg	977.85	J/mol×K	908.78	Joback Method
cpg	962.66	J/mol×K	877.82	Joback Method
cpg	946.44	J/mol×K	846.86	Joback Method
cpg	929.17	J/mol×K	815.90	Joback Method
cpg	1005.19	J/mol×K	970.70	Joback Method
dvisc	0.0000439	Pa×s	784.94	Joback Method

dvisc	0.0000624	Pa×s	718.82	Joback Method
dvisc	0.0000950	Pa×s	652.70	Joback Method
dvisc	0.0001591	Pa×s	586.58	Joback Method
dvisc	0.0003040	Pa×s	520.45	Joback Method
dvisc	0.0007008	Pa×s	454.33	Joback Method
dvisc	0.0021477	Pa×s	388.21	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349779&Units=SI

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

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