Adipic acid, 3,3-dimethylbut-2-yl heptyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-358.34	kJ/mol	Joback Method
hf	-939.12	kJ/mol	Joback Method
hfus	39.60	kJ/mol	Joback Method
hvap	74.52	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	5.038		Crippen Method
mcvol	293.450	ml/mol	McGowan Method
pc	1170.42	kPa	Joback Method
rinpol	2106.00		NIST Webbook
tb	783.03	K	Joback Method
tc	968.31	K	Joback Method
tf	435.63	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.66	J/mol×K	783.03	Joback Method
cpg	990.82	J/mol×K	937.43	Joback Method
cpg	976.73	J/mol×K	906.55	Joback Method
cpg	961.70	J/mol×K	875.67	Joback Method
cpg	945.69	J/mol×K	844.79	Joback Method
cpg	928.69	J/mol×K	813.91	Joback Method
cpg	1004.00	J/mol×K	968.31	Joback Method
dvisc	0.0000457	Pa×s	783.03	Joback Method
dvisc	0.0000628	Pa×s	725.13	Joback Method

dvisc	0.0000912	Pa×s	667.23	Joback Method
dvisc	0.0001421	Pa×s	609.33	Joback Method
dvisc	0.0002430	Pa×s	551.43	Joback Method
dvisc	0.0004713	Pa×s	493.53	Joback Method
dvisc	0.0010903	Pa×s	435.63	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=U353672&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

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