

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

Inchi:	InChI=1S/C17H32O4/c1-12(2)11-20-15(18)9-7-8-10-16(19)21-17(13(3)4)14(5)6/h12-14,1
InchiKey:	SRIUMBSREUVAGZ-UHFFFAOYSA-N
Formula:	C17H32O4
SMILES:	CC(C)COC(=O)CCCC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]:	300.43

Physical Properties

Property code	Value	Unit	Source
gf	-385.34	kJ/mol	Joback Method
hf	-904.93	kJ/mol	Joback Method
hfus	31.27	kJ/mol	Joback Method
hvap	70.20	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.970		Crippen Method
mvol	265.270	ml/mol	McGowan Method
pc	1345.70	kPa	Joback Method
rinpol	1862.00		NIST Webbook
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tb	739.18	K	Joback Method
tc	923.55	K	Joback Method
tf	365.67	K	Joback Method
vc	1.012	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.97	J/molxK	739.18	Joback Method
cpg	872.12	J/molxK	892.82	Joback Method
cpg	858.18	J/molxK	862.09	Joback Method
cpg	843.31	J/molxK	831.36	Joback Method
cpg	827.49	J/molxK	800.64	Joback Method
cpg	810.71	J/molxK	769.91	Joback Method
cpg	885.13	J/molxK	923.55	Joback Method
dvisc	0.0000587	Paxs	739.18	Joback Method

dvisc	0.0000831	Paxs	676.93	Joback Method
dvisc	0.0001264	Paxs	614.68	Joback Method
dvisc	0.0002111	Paxs	552.42	Joback Method
dvisc	0.0004018	Paxs	490.17	Joback Method
dvisc	0.0009221	Paxs	427.92	Joback Method
dvisc	0.0028079	Paxs	365.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349776&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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