

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

Inchi:	InChI=1S/C14H26O4/c1-6-17-12(15)9-7-8-10-13(16)18-11(2)14(3,4)5/h11H,6-10H2,1-5H
InchiKey:	OTUGUVVYACOZQL-UHFFFAOYSA-N
Formula:	C14H26O4
SMILES:	CCOC(=O)CCCC(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]:	258.35

Physical Properties

Property code	Value	Unit	Source
gf	-400.44	kJ/mol	Joback Method
hf	-835.92	kJ/mol	Joback Method
hfus	26.65	kJ/mol	Joback Method
hvap	63.39	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	3.088		Crippen Method
mcvol	223.000	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
rinqol	1620.00		NIST Webbook
tb	668.63	K	Joback Method
tc	854.31	K	Joback Method
tf	379.28	K	Joback Method
vc	0.851	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.23	J/molxK	668.63	Joback Method
cpg	641.58	J/molxK	699.58	Joback Method
cpg	657.08	J/molxK	730.52	Joback Method
cpg	671.74	J/molxK	761.47	Joback Method
cpg	685.59	J/molxK	792.42	Joback Method
cpg	698.63	J/molxK	823.36	Joback Method
cpg	710.90	J/molxK	854.31	Joback Method
dvisc	0.0019390	Paxs	379.28	Joback Method
dvisc	0.0008833	Paxs	427.50	Joback Method

dvisc	0.0004719	Paxs	475.73	Joback Method
dvisc	0.0002830	Paxs	523.96	Joback Method
dvisc	0.0001849	Paxs	572.18	Joback Method
dvisc	0.0001291	Paxs	620.40	Joback Method
dvisc	0.0000950	Paxs	668.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353665&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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