

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

Inchi:	InChI=1S/C15H28O4/c1-6-18-13(16)9-7-8-10-14(17)19-15(11(2)3)12(4)5/h11-12,15H,6-
InchiKey:	IZSXMOQPGJLKDG-UHFFFAOYSA-N
Formula:	C15H28O4
SMILES:	CCOC(=O)CCCC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]:	272.38

Physical Properties

Property code	Value	Unit	Source
gf	-399.74	kJ/mol	Joback Method
hf	-858.37	kJ/mol	Joback Method
hfus	29.61	kJ/mol	Joback Method
hvap	66.13	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.334		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1547.57	kPa	Joback Method
rinpol	1717.00		NIST Webbook
rinpol	1717.00		NIST Webbook
tb	693.86	K	Joback Method
tc	876.51	K	Joback Method
tf	358.13	K	Joback Method
vc	0.905	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.70	J/molxK	693.86	Joback Method
cpg	695.52	J/molxK	724.30	Joback Method
cpg	711.49	J/molxK	754.74	Joback Method
cpg	726.61	J/molxK	785.18	Joback Method
cpg	740.89	J/molxK	815.62	Joback Method
cpg	754.34	J/molxK	846.06	Joback Method
cpg	766.97	J/molxK	876.51	Joback Method
dvisc	0.0027078	Paxs	358.13	Joback Method

dvisc	0.0010257	Paxs	414.08	Joback Method
dvisc	0.0004895	Paxs	470.04	Joback Method
dvisc	0.0002735	Paxs	526.00	Joback Method
dvisc	0.0001709	Paxs	581.95	Joback Method
dvisc	0.0001159	Paxs	637.90	Joback Method
dvisc	0.0000837	Paxs	693.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349775&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
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

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