

Adipic acid, hexyl 3-oxobut-2-yl ester

Inchi:	InChI=1S/C16H28O5/c1-4-5-6-9-12-20-15(18)10-7-8-11-16(19)21-14(3)13(2)17/h14H,4-
InchiKey:	REZVKAGCPPLRHT-UHFFFAOYSA-N
Formula:	C16H28O5
SMILES:	CCCCCOC(=O)CCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]:	300.39

Physical Properties

Property code	Value	Unit	Source
gf	-515.36	kJ/mol	Joback Method
hf	-981.03	kJ/mol	Joback Method
hfus	40.85	kJ/mol	Joback Method
hvap	75.88	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.191		Crippen Method
mvol	252.750	ml/mol	McGowan Method
pc	1489.58	kPa	Joback Method
rinpol	2025.00		NIST Webbook
rinpol	2025.00		NIST Webbook
tb	771.49	K	Joback Method
tc	957.72	K	Joback Method
tf	449.33	K	Joback Method
vc	0.980	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.61	J/molxK	771.49	Joback Method
cpg	772.06	J/molxK	802.53	Joback Method
cpg	786.59	J/molxK	833.57	Joback Method
cpg	800.23	J/molxK	864.60	Joback Method
cpg	812.97	J/molxK	895.64	Joback Method
cpg	824.83	J/molxK	926.68	Joback Method
cpg	835.81	J/molxK	957.72	Joback Method
dvisc	0.0011537	Paxs	449.33	Joback Method

dvisc	0.0005879	Paxs	503.02	Joback Method
dvisc	0.0003412	Paxs	556.72	Joback Method
dvisc	0.0002179	Paxs	610.41	Joback Method
dvisc	0.0001497	Paxs	664.10	Joback Method
dvisc	0.0001087	Paxs	717.80	Joback Method
dvisc	0.0000826	Paxs	771.49	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=U353750&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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