

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

Inchi:	InChI=1S/C21H38O5/c1-4-5-6-7-8-9-10-11-14-17-25-20(23)15-12-13-16-21(24)26-19(3)
InchiKey:	YTWYGDOTSPNSLD-UHFFFAOYSA-N
Formula:	C21H38O5
SMILES:	CCCCCCCCCOC(=O)CCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]:	370.52

Physical Properties

Property code	Value	Unit	Source
gf	-473.26	kJ/mol	Joback Method
hf	-1084.23	kJ/mol	Joback Method
hfus	53.80	kJ/mol	Joback Method
hvap	87.01	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	5.141		Crippen Method
mvol	323.200	ml/mol	McGowan Method
pc	1060.33	kPa	Joback Method
rinpol	2526.00		NIST Webbook
rinpol	2526.00		NIST Webbook
tb	885.89	K	Joback Method
tc	1084.76	K	Joback Method
tf	505.68	K	Joback Method
vc	1.260	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1053.22	J/molxK	885.89	Joback Method
cpg	1070.44	J/molxK	919.03	Joback Method
cpg	1086.42	J/molxK	952.18	Joback Method
cpg	1101.18	J/molxK	985.32	Joback Method
cpg	1114.75	J/molxK	1018.47	Joback Method
cpg	1127.14	J/molxK	1051.61	Joback Method
cpg	1138.39	J/molxK	1084.76	Joback Method
dvisc	0.0006604	Paxs	505.68	Joback Method

dvisc	0.0003187	Paxs	569.05	Joback Method
dvisc	0.0001780	Paxs	632.42	Joback Method
dvisc	0.0001105	Paxs	695.78	Joback Method
dvisc	0.0000743	Paxs	759.15	Joback Method
dvisc	0.0000531	Paxs	822.52	Joback Method
dvisc	0.0000398	Paxs	885.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353755&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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