

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

Inchi:	InChI=1S/C20H36O5/c1-4-5-6-7-8-9-10-13-16-24-19(22)14-11-12-15-20(23)25-18(3)17(2)
InchiKey:	SSIZTQUREVCLPS-UHFFFAOYSA-N
Formula:	C20H36O5
SMILES:	CCCCCCCCCOC(=O)CCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]:	356.50

Physical Properties

Property code	Value	Unit	Source
gf	-481.68	kJ/mol	Joback Method
hf	-1063.59	kJ/mol	Joback Method
hfus	51.21	kJ/mol	Joback Method
hvap	84.78	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.751		Crippen Method
mcvol	309.110	ml/mol	McGowan Method
pc	1129.86	kPa	Joback Method
rinsol	2430.00		NIST Webbook
tb	863.01	K	Joback Method
tc	1057.77	K	Joback Method
tf	494.41	K	Joback Method
vc	1.204	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	992.39	J/molxK	863.01	Joback Method
cpg	1065.27	J/molxK	1025.31	Joback Method
cpg	1052.93	J/molxK	992.85	Joback Method
cpg	1039.49	J/molxK	960.39	Joback Method
cpg	1024.93	J/molxK	927.93	Joback Method
cpg	1009.24	J/molxK	895.47	Joback Method
cpg	1076.52	J/molxK	1057.77	Joback Method
dvisc	0.0000463	Paxs	863.01	Joback Method
dvisc	0.0000616	Paxs	801.58	Joback Method

dvisc	0.0000859	Paxs	740.14	Joback Method
dvisc	0.0001273	Paxs	678.71	Joback Method
dvisc	0.0002040	Paxs	617.28	Joback Method
dvisc	0.0003626	Paxs	555.84	Joback Method
dvisc	0.0007439	Paxs	494.41	Joback Method

Sources

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=U353754&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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