

Adipic acid, pent-4-enyl undecyl ester

Inchi:	InChI=1S/C22H40O4/c1-3-5-7-8-9-10-11-12-16-20-26-22(24)18-14-13-17-21(23)25-19-1
InchiKey:	IXTSOFLLTXSSRH-UHFFFAOYSA-N
Formula:	C22H40O4
SMILES:	C=CCCCOC(=O)CCCCC(=O)OCCCCCCCCCCC
Mol. weight [g/mol]:	368.55

Physical Properties

Property code	Value	Unit	Source
gf	-245.64	kJ/mol	Joback Method
hf	-861.58	kJ/mol	Joback Method
hfus	57.03	kJ/mol	Joback Method
hvap	82.21	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	6.130		Crippen Method
mcvol	331.420	ml/mol	McGowan Method
pc	979.01	kPa	Joback Method
rinpol	2528.00		NIST Webbook
tb	852.02	K	Joback Method
tc	1043.34	K	Joback Method
tf	480.26	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1064.09	J/molxK	852.02	Joback Method
cpg	1082.68	J/molxK	883.91	Joback Method
cpg	1100.12	J/molxK	915.79	Joback Method
cpg	1116.44	J/molxK	947.68	Joback Method
cpg	1131.66	J/molxK	979.56	Joback Method
cpg	1145.82	J/molxK	1011.45	Joback Method
cpg	1158.94	J/molxK	1043.34	Joback Method
dvisc	0.0006825	Paxs	480.26	Joback Method
dvisc	0.0003301	Paxs	542.22	Joback Method

dvisc	0.0001853	Paxs	604.18	Joback Method
dvisc	0.0001158	Paxs	666.14	Joback Method
dvisc	0.0000784	Paxs	728.10	Joback Method
dvisc	0.0000564	Paxs	790.06	Joback Method
dvisc	0.0000426	Paxs	852.02	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=U353800&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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