

Adipic acid, octyl trans-hex-3-enyl ester

Inchi:	InChI=1S/C20H36O4/c1-3-5-7-9-10-14-18-24-20(22)16-12-11-15-19(21)23-17-13-8-6-4-2
InchiKey:	XWTRADSAYBWLTM-SOFGYWHQSA-N
Formula:	C20H36O4
SMILES:	CCC=CCCOC(=O)CCCCC(=O)OCCCCCCCC
Mol. weight [g/mol]:	340.50

Physical Properties

Property code	Value	Unit	Source
gf	-270.10	kJ/mol	Joback Method
hf	-828.51	kJ/mol	Joback Method
hfus	53.33	kJ/mol	Joback Method
hvap	78.38	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	5.350		Crippen Method
mcvol	303.240	ml/mol	McGowan Method
pc	1115.57	kPa	Joback Method
rinsol	2328.00		NIST Webbook
tb	813.74	K	Joback Method
tc	999.86	K	Joback Method
tf	454.40	K	Joback Method
vc	1.183	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	943.87	J/molxK	813.74	Joback Method
cpg	961.55	J/molxK	844.76	Joback Method
cpg	978.23	J/molxK	875.78	Joback Method
cpg	993.95	J/molxK	906.80	Joback Method
cpg	1008.72	J/molxK	937.82	Joback Method
cpg	1022.58	J/molxK	968.84	Joback Method
cpg	1035.55	J/molxK	999.86	Joback Method
dvisc	0.0007807	Paxs	454.40	Joback Method
dvisc	0.0003707	Paxs	514.29	Joback Method

dvisc	0.0002056	Paxs	574.18	Joback Method
dvisc	0.0001274	Paxs	634.07	Joback Method
dvisc	0.0000858	Paxs	693.96	Joback Method
dvisc	0.0000615	Paxs	753.85	Joback Method
dvisc	0.0000463	Paxs	813.74	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=U354012&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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