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
rinpol	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0002056	Pa×s	574.18	Joback Method
dvisc	0.0001274	Pa×s	634.07	Joback Method
dvisc	0.0000858	Pa×s	693.96	Joback Method
dvisc	0.0000615	Pa×s	753.85	Joback Method
dvisc	0.0000463	Pa×s	813.74	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U354012&Units=SI

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