Adipic acid, octyl pent-4-en-2-yl ester

Inchi: InChI=1S/C19H34O4/c1-4-6-7-8-9-12-16-22-18(20)14-10-11-15-19(21)23-17(3)13-5-2/h5
InchiKey: IOXXCUCRKDPOBB-UHFFFAOYSA-N
Formula: C19H34O4
SMILES: C=CCC(C)OC(=O)CCCCC(=O)OCCCCCCCC
Mol. weight [g/mol]: 326.47

Physical Properties

Property code	Value	Unit	Source
gf	-273.34	kJ/mol	Joback Method
hf	-804.94	kJ/mol	Joback Method
hfus	45.74	kJ/mol	Joback Method
hvap	75.14	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	4.958		Crippen Method
mcvol	289.150	ml/mol	McGowan Method
pc	1189.06	kPa	Joback Method
rinpol	2148.00		NIST Webbook
tb	782.94	K	Joback Method
tc	965.60	K	Joback Method
tf	431.45	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	883.01	J/mol×K	782.94	Joback Method
cpg	900.42	J/mol×K	813.38	Joback Method
cpg	916.86	J/mol×K	843.83	Joback Method
cpg	932.34	J/mol×K	874.27	Joback Method
cpg	946.90	J/mol×K	904.71	Joback Method
cpg	960.54	J/mol×K	935.16	Joback Method
cpg	973.28	J/mol×K	965.60	Joback Method
dvisc	0.0011185	Pa×s	431.45	Joback Method
dvisc	0.0005136	Pa×s	490.03	Joback Method

dvisc	0.0002785	Pa×s	548.61	Joback Method
dvisc	0.0001700	Pa×s	607.20	Joback Method
dvisc	0.0001131	Pa×s	665.78	Joback Method
dvisc	0.0000804	Pa×s	724.36	Joback Method
dvisc	0.0000602	Pa×s	782.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354124&Units=SI
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

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