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

Inchi: InChI=1S/C22H40O4/c1-4-6-7-8-9-10-11-12-15-19-25-21(23)17-13-14-18-22(24)26-20(3
InchiKey: ZBTQYMQDXDFQDB-UHFFFAOYSA-N
Formula: C22H40O4
SMILES: C=CCC(C)OC(=O)CCCCC(=O)OCCCCCCCCCCC
Mol. weight [g/mol]: 368.55

Physical Properties

Property code	Value	Unit	Source
gf	-248.08	kJ/mol	Joback Method
hf	-866.86	kJ/mol	Joback Method
hfus	53.51	kJ/mol	Joback Method
hvap	81.82	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	6.129		Crippen Method
mcvol	331.420	ml/mol	McGowan Method
pc	983.93	kPa	Joback Method
rinpol	2447.00		NIST Webbook
tb	851.58	K	Joback Method
tc	1043.11	K	Joback Method
tf	465.26	K	Joback Method
vc	1.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1064.56	J/mol×K	851.58	Joback Method
cpg	1083.16	J/mol×K	883.50	Joback Method
cpg	1100.60	J/mol×K	915.42	Joback Method
cpg	1116.90	J/mol×K	947.35	Joback Method
cpg	1132.10	J/mol×K	979.27	Joback Method
cpg	1146.23	J/mol×K	1011.19	Joback Method
cpg	1159.30	J/mol×K	1043.11	Joback Method
dvisc	0.0007948	Pa×s	465.26	Joback Method
dvisc	0.0003544	Pa×s	529.65	Joback Method

dvisc	0.0001883	Pa×s	594.03	Joback Method
dvisc	0.0001132	Pa×s	658.42	Joback Method
dvisc	0.0000745	Pa×s	722.81	Joback Method
dvisc	0.0000525	Pa×s	787.19	Joback Method
dvisc	0.0000390	Pa×s	851.58	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=U354127&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

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