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

Inchi: InChI=1S/C28H52O4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-21-25-31-27(29)23-19-2
InchiKey: DRWYHQDBJBSZMR-UHFFFAOYSA-N
Formula: C28H52O4
SMILES: C=CCC(C)OC(=O)CCCCC(=O)OCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 452.71

Physical Properties

Property code	Value	Unit	Source
gf	-197.56	kJ/mol	Joback Method
hf	-990.70	kJ/mol	Joback Method
hfus	69.05	kJ/mol	Joback Method
hvap	95.18	kJ/mol	Joback Method
log10ws	-9.23		Crippen Method
logp	8.469		Crippen Method
mcvol	415.960	ml/mol	McGowan Method
pc	705.83	kPa	Joback Method
rinpol	3051.00		NIST Webbook
tb	988.86	K	Joback Method
tc	1223.54	K	Joback Method
tf	532.88	K	Joback Method
vc	1.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1444.53	J/mol×K	988.86	Joback Method
cpg	1535.66	J/mol×K	1184.43	Joback Method
cpg	1520.89	J/mol×K	1145.31	Joback Method
cpg	1504.47	J/mol×K	1106.20	Joback Method
cpg	1486.32	J/mol×K	1067.09	Joback Method
cpg	1466.36	J/mol×K	1027.97	Joback Method
cpg	1548.85	J/mol×K	1223.54	Joback Method
dvisc	0.0000155	Pa×s	988.86	Joback Method
dvisc	0.0000211	Pa×s	912.86	Joback Method

dvisc	0.0000304	Pa×s	836.87	Joback Method
dvisc	0.0000470	Pa×s	760.87	Joback Method
dvisc	0.0000802	Pa×s	684.87	Joback Method
dvisc	0.0001561	Pa×s	608.88	Joback Method
dvisc	0.0003676	Pa×s	532.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354132&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

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