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

Inchi: InChI=1S/C26H48O4/c1-4-6-7-8-9-10-11-12-13-14-15-16-19-23-29-25(27)21-17-18-22-2
InchiKey: ZDTBGLOFVDYWHH-UHFFFAOYSA-N
Formula: C26H48O4
SMILES: C=CCC(C)OC(=O)CCCCC(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 424.66

Physical Properties

Property code	Value	Unit	Source
gf	-214.40	kJ/mol	Joback Method
hf	-949.42	kJ/mol	Joback Method
hfus	63.87	kJ/mol	Joback Method
hvap	90.72	kJ/mol	Joback Method
log10ws	-8.40		Crippen Method
logp	7.689		Crippen Method
mcvol	387.780	ml/mol	McGowan Method
pc	783.75	kPa	Joback Method
rinpol	2847.00		NIST Webbook
rinpol	2847.00		NIST Webbook
tb	943.10	K	Joback Method
tc	1158.91	K	Joback Method
tf	510.34	K	Joback Method
vc	1.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1315.93	J/mol×K	943.10	Joback Method
cpg	1403.66	J/mol×K	1122.94	Joback Method
cpg	1389.04	J/mol×K	1086.97	Joback Method
cpg	1373.01	J/mol×K	1051.01	Joback Method
cpg	1355.52	J/mol×K	1015.04	Joback Method
cpg	1336.51	J/mol×K	979.07	Joback Method
cpg	1416.91	J/mol×K	1158.91	Joback Method
dvisc	0.0000213	Pa×s	943.10	Joback Method

dvisc	0.0000288	Pa×s	870.97	Joback Method
dvisc	0.0000413	Pa×s	798.85	Joback Method
dvisc	0.0000635	Pa×s	726.72	Joback Method
dvisc	0.0001075	Pa×s	654.59	Joback Method
dvisc	0.0002072	Pa×s	582.47	Joback Method
dvisc	0.0004805	Pa×s	510.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354130&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