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

Inchi: InChI=1S/C25H46O4/c1-4-6-7-8-9-10-11-12-13-14-15-18-22-28-24(26)20-16-17-21-25(2
InchiKey: OXDUNNYAJCNRRV-UHFFFAOYSA-N
Formula: C25H46O4
SMILES: C=CCC(C)OC(=O)CCCCC(=O)OCCCCCCCCCCCCCC
Mol. weight [g/mol]: 410.63

Physical Properties

Property code	Value	Unit	Source
gf	-222.82	kJ/mol	Joback Method
hf	-928.78	kJ/mol	Joback Method
hfus	61.28	kJ/mol	Joback Method
hvap	88.50	kJ/mol	Joback Method
log10ws	-7.98		Crippen Method
logp	7.299		Crippen Method
mcvol	373.690	ml/mol	McGowan Method
pc	827.64	kPa	Joback Method
rinpol	2744.00		NIST Webbook
tb	920.22	K	Joback Method
tc	1128.41	K	Joback Method
tf	499.07	K	Joback Method
vc	1.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1252.27	J/mol×K	920.22	Joback Method
cpg	1272.30	J/mol×K	954.92	Joback Method
cpg	1290.88	J/mol×K	989.62	Joback Method
cpg	1308.06	J/mol×K	1024.31	Joback Method
cpg	1323.89	J/mol×K	1059.01	Joback Method
cpg	1338.40	J/mol×K	1093.71	Joback Method
cpg	1351.64	J/mol×K	1128.41	Joback Method
dvisc	0.0005474	Pa×s	499.07	Joback Method
dvisc	0.0002378	Pa×s	569.26	Joback Method

dvisc	0.0001241	Pa×s	639.45	Joback Method
dvisc	0.0000736	Pa×s	709.64	Joback Method
dvisc	0.0000480	Pa×s	779.84	Joback Method
dvisc	0.0000336	Pa×s	850.03	Joback Method
dvisc	0.0000248	Pa×s	920.22	Joback Method

Sources

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=U354129&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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