Adipic acid, trans-hex-3-enyl tridecyl ester

Inchi: InChI=1S/C25H46O4/c1-3-5-7-9-10-11-12-13-14-15-19-23-29-25(27)21-17-16-20-24(26)28-22-18-8-6-4-2
InchiKey: ORDSDMDWUAZDNZ-SOFGYWHQSA-N
Formula: C25H46O4
SMILES: CCC=CCCOC(=O)CCCCC(=O)OCCCCCCCCCCCCC
Mol. weight [g/mol]: 410.63

Physical Properties

Property code	Value	Unit	Source
gf	-228.00	kJ/mol	Joback Method
hf	-931.71	kJ/mol	Joback Method
hfus	66.28	kJ/mol	Joback Method
hvap	89.51	kJ/mol	Joback Method
log10ws	-7.87		Crippen Method
logp	7.300		Crippen Method
mcvol	373.690	ml/mol	McGowan Method
pc	828.59	kPa	Joback Method
rinpol	2824.00		NIST Webbook
tb	928.14	K	Joback Method
tc	1138.56	K	Joback Method
tf	510.75	K	Joback Method
vc	1.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1253.80	J/mol×K	928.14	Joback Method
cpg	1273.93	J/mol×K	963.21	Joback Method
cpg	1292.67	J/mol×K	998.28	Joback Method
cpg	1310.08	J/mol×K	1033.35	Joback Method
cpg	1326.20	J/mol×K	1068.42	Joback Method
cpg	1341.10	J/mol×K	1103.49	Joback Method
cpg	1354.81	J/mol×K	1138.56	Joback Method
dvisc	0.0004320	Pa×s	510.75	Joback Method
dvisc	0.0001956	Pa×s	580.31	Joback Method

dvisc	0.0001049	Pa×s	649.88	Joback Method
dvisc	0.0000635	Pa×s	719.44	Joback Method
dvisc	0.0000420	Pa×s	789.01	Joback Method
dvisc	0.0000297	Pa×s	858.58	Joback Method
dvisc	0.0000221	Pa×s	928.14	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=U354017&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