Adipic acid, cis-hex-3-enyl hexadecyl ester

Inchi: InChI=1S/C28H52O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-22-26-32-28(30)24-20-19-
InchiKey: VFOCHYXWAFNOGA-VURMDHGXSA-N
Formula: C28H52O4
SMILES: CCC=CCCOC(=O)CCCCC(=O)OCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 452.71

Physical Properties

Property code	Value	Unit	Source
gf	-202.74	kJ/mol	Joback Method
hf	-993.63	kJ/mol	Joback Method
hfus	74.05	kJ/mol	Joback Method
hvap	96.19	kJ/mol	Joback Method
log10ws	-9.12		Crippen Method
logp	8.471		Crippen Method
mcvol	415.960	ml/mol	McGowan Method
pc	706.58	kPa	Joback Method
rinpol	3146.00		NIST Webbook
rinpol	3146.00		NIST Webbook
tb	996.78	K	Joback Method
tc	1234.53	K	Joback Method
tf	544.56	K	Joback Method
vc	1.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1446.46	J/mol×K	996.78	Joback Method
cpg	1468.63	J/mol×K	1036.40	Joback Method
cpg	1489.00	J/mol×K	1076.03	Joback Method
cpg	1507.66	J/mol×K	1115.65	Joback Method
cpg	1524.71	J/mol×K	1155.28	Joback Method
cpg	1540.23	J/mol×K	1194.90	Joback Method
cpg	1554.32	J/mol×K	1234.53	Joback Method
dvisc	0.0002922	Pa×s	544.56	Joback Method

dvisc	0.0001291	Pa×s	619.93	Joback Method
dvisc	0.0000681	Pa×s	695.30	Joback Method
dvisc	0.0000407	Pa×s	770.67	Joback Method
dvisc	0.0000266	Pa×s	846.04	Joback Method
dvisc	0.0000187	Pa×s	921.41	Joback Method
dvisc	0.0000139	Pa×s	996.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353984&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