Fumaric acid, cis-hex-3-enyl tridecyl ester

Inchi: InChI=1S/C23H40O4/c1-3-5-7-9-10-11-12-13-14-15-17-21-27-23(25)19-18-22(24)26-20-
InchiKey: NWYSCFQMVILLBL-JCNZJEDXSA-N
Formula: C23H40O4
SMILES: CCC=CCCOC(=O)C=CC(=O)OCCCCCCCCCCCCC
Mol. weight [g/mol]: 380.56

Physical Properties

Property code	Value	Unit	Source
gf	-164.62	kJ/mol	Joback Method
hf	-773.21	kJ/mol	Joback Method
hfus	61.30	kJ/mol	Joback Method
hvap	85.02	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	6.296		Crippen Method
mcvol	341.210	ml/mol	McGowan Method
pc	958.51	kPa	Joback Method
rinpol	2690.00		NIST Webbook
rinpol	2690.00		NIST Webbook
tb	886.54	K	Joback Method
tc	1085.50	K	Joback Method
tf	483.13	K	Joback Method
vc	1.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1101.05	J/mol×K	886.54	Joback Method
cpg	1182.89	J/mol×K	1052.34	Joback Method
cpg	1168.53	J/mol×K	1019.18	Joback Method
cpg	1153.22	J/mol×K	986.02	Joback Method
cpg	1136.90	J/mol×K	952.86	Joback Method
cpg	1119.53	J/mol×K	919.70	Joback Method
cpg	1196.35	J/mol×K	1085.50	Joback Method
dvisc	0.0000261	Pa×s	886.54	Joback Method

dvisc	0.0000350	Pa×s	819.31	Joback Method
dvisc	0.0000494	Pa×s	752.07	Joback Method
dvisc	0.0000747	Pa×s	684.84	Joback Method
dvisc	0.0001236	Pa×s	617.60	Joback Method
dvisc	0.0002312	Pa×s	550.37	Joback Method
dvisc	0.0005147	Pa×s	483.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348868&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