Fumaric acid, 3-hexyl tridecyl ester

Inchi: InChI=1S/C23H42O4/c1-4-7-8-9-10-11-12-13-14-15-16-20-26-22(24)18-19-23(25)27-21(
InchiKey: MVOXLTNOMWSALX-VHEBQXMUSA-N
Formula: C23H42O4
SMILES: CCCCCCCCCCCCCOC(=O)C=CC(=O)OC(CC)CCC
Mol. weight [g/mol]: 382.58

Physical Properties

Property code	Value	Unit	Source
gf	-247.28	kJ/mol	Joback Method
hf	-895.71	kJ/mol	Joback Method
hfus	57.58	kJ/mol	Joback Method
hvap	84.67	kJ/mol	Joback Method
log10ws	-7.14		Crippen Method
logp	6.519		Crippen Method
mcvol	345.510	ml/mol	McGowan Method
pc	932.92	kPa	Joback Method
rinpol	2593.00		NIST Webbook
tb	881.94	K	Joback Method
tc	1079.77	K	Joback Method
tf	473.21	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1128.31	J/mol×K	881.94	Joback Method
cpg	1147.33	J/mol×K	914.91	Joback Method
cpg	1165.14	J/mol×K	947.88	Joback Method
cpg	1181.78	J/mol×K	980.86	Joback Method
cpg	1197.28	J/mol×K	1013.83	Joback Method
cpg	1211.70	J/mol×K	1046.80	Joback Method
cpg	1225.06	J/mol×K	1079.77	Joback Method
dvisc	0.0006444	Pa×s	473.21	Joback Method
dvisc	0.0002732	Pa×s	541.33	Joback Method

dvisc	0.0001403	Pa×s	609.45	Joback Method
dvisc	0.0000824	Pa×s	677.58	Joback Method
dvisc	0.0000533	Pa×s	745.70	Joback Method
dvisc	0.0000371	Pa×s	813.82	Joback Method
dvisc	0.0000273	Pa×s	881.94	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=U348612&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