Fumaric acid, hexyl tetradec-3-enyl ester

Inchi: InChI=1S/C24H42O4/c1-3-5-7-9-10-11-12-13-14-15-16-18-22-28-24(26)20-19-23(25)27-
InchiKey: UXDMUNOWESHSTL-LMOVRVBNSA-N
Formula: C24H42O4
SMILES: CCCCCCCCCCC=CCCOC(=O)C=CC(=O)OCCCCCC
Mol. weight [g/mol]: 394.59

Physical Properties

Property code	Value	Unit	Source
gf	-156.20	kJ/mol	Joback Method
hf	-793.85	kJ/mol	Joback Method
hfus	63.89	kJ/mol	Joback Method
hvap	87.25	kJ/mol	Joback Method
log10ws	-7.30		Crippen Method
logp	6.686		Crippen Method
mcvol	355.300	ml/mol	McGowan Method
pc	903.97	kPa	Joback Method
rinpol	2790.00		NIST Webbook
rinpol	2790.00		NIST Webbook
tb	909.42	K	Joback Method
tc	1113.50	K	Joback Method
tf	494.40	K	Joback Method
vc	1.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1163.37	J/mol×K	909.42	Joback Method
cpg	1182.36	J/mol×K	943.43	Joback Method
cpg	1200.19	J/mol×K	977.45	Joback Method
cpg	1216.90	J/mol×K	1011.46	Joback Method
cpg	1232.55	J/mol×K	1045.48	Joback Method
cpg	1247.20	J/mol×K	1079.49	Joback Method
cpg	1260.91	J/mol×K	1113.50	Joback Method
dvisc	0.0004557	Pa×s	494.40	Joback Method

dvisc	0.0002029	Pa×s	563.57	Joback Method
dvisc	0.0001078	Pa×s	632.74	Joback Method
dvisc	0.0000649	Pa×s	701.91	Joback Method
dvisc	0.0000428	Pa×s	771.08	Joback Method
dvisc	0.0000302	Pa×s	840.25	Joback Method
dvisc	0.0000225	Pa×s	909.42	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348837&Units=SI

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