Fumaric acid, isohexyl tetradec-3-enyl ester

Inchi: InChI=1S/C24H42O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-20-27-23(25)18-19-24(26)28-21
InchiKey: ROQXFWBMOPKROI-CDSOMVEVSA-N
Formula: C24H42O4
SMILES: CCCCCCCCCCC=CCCOC(=O)C=CC(=O)OCCCC(C)C
Mol. weight [g/mol]: 394.59

Physical Properties

Property code	Value	Unit	Source
gf	-158.64	kJ/mol	Joback Method
hf	-799.13	kJ/mol	Joback Method
hfus	60.37	kJ/mol	Joback Method
hvap	86.86	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	6.542		Crippen Method
mcvol	355.300	ml/mol	McGowan Method
pc	908.34	kPa	Joback Method
rinpol	2749.00		NIST Webbook
rinpol	2749.00		NIST Webbook
tb	908.98	K	Joback Method
tc	1112.85	K	Joback Method
tf	479.40	K	Joback Method
vc	1.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1163.79	J/mol×K	908.98	Joback Method
cpg	1182.74	J/mol×K	942.96	Joback Method
cpg	1200.51	J/mol×K	976.94	Joback Method
cpg	1217.15	J/mol×K	1010.92	Joback Method
cpg	1232.73	J/mol×K	1044.89	Joback Method
cpg	1247.29	J/mol×K	1078.87	Joback Method
cpg	1260.91	J/mol×K	1112.85	Joback Method
dvisc	0.0005301	Pa×s	479.40	Joback Method

dvisc	0.0002169	Pa×s	551.00	Joback Method
dvisc	0.0001090	Pa×s	622.59	Joback Method
dvisc	0.0000631	Pa×s	694.19	Joback Method
dvisc	0.0000405	Pa×s	765.79	Joback Method
dvisc	0.0000280	Pa×s	837.38	Joback Method
dvisc	0.0000205	Pa×s	908.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348836&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

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