Fumaric acid, octadecyl trans-hex-3-enyl ester

Inchi: InChI=1S/C28H50O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-19-20-22-26-32-28(30)24-
InchiKey: GYXYRKFEGBVEOO-FYTAZISXSA-N
Formula: C28H50O4
SMILES: CCC=CCCOC(=O)C=CC(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 450.69

Physical Properties

Property code	Value	Unit	Source
gf	-122.52	kJ/mol	Joback Method
hf	-876.41	kJ/mol	Joback Method
hfus	74.25	kJ/mol	Joback Method
hvap	96.15	kJ/mol	Joback Method
log10ws	-8.98		Crippen Method
logp	8.247		Crippen Method
mcvol	411.660	ml/mol	McGowan Method
pc	726.53	kPa	Joback Method
rinpol	3177.00		NIST Webbook
tb	1000.94	K	Joback Method
tc	1236.34	K	Joback Method
tf	539.48	K	Joback Method
vc	1.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1418.29	J/mol×K	1000.94	Joback Method
cpg	1439.94	J/mol×K	1040.17	Joback Method
cpg	1460.04	J/mol×K	1079.41	Joback Method
cpg	1478.68	J/mol×K	1118.64	Joback Method
cpg	1495.98	J/mol×K	1157.87	Joback Method
cpg	1512.04	J/mol×K	1197.11	Joback Method
cpg	1526.96	J/mol×K	1236.34	Joback Method
dvisc	0.0002721	Pa×s	539.48	Joback Method
dvisc	0.0001173	Pa×s	616.39	Joback Method

dvisc	0.0000610	Pa×s	693.30	Joback Method
dvisc	0.0000361	Pa×s	770.21	Joback Method
dvisc	0.0000235	Pa×s	847.12	Joback Method
dvisc	0.0000165	Pa×s	924.03	Joback Method
dvisc	0.0000122	Pa×s	1000.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348898&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