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

Inchi: InChI=1S/C18H30O4/c1-3-5-7-9-10-12-16-22-18(20)14-13-17(19)21-15-11-8-6-4-2/h6,8,
InchiKey: CSLQNKVIOMWFJK-INQIEHEISA-N
Formula: C18H30O4
SMILES: CCC=CCCOC(=O)C=CC(=O)OCCCCCCCC
Mol. weight [g/mol]: 310.43

Physical Properties

Property code	Value	Unit	Source
gf	-206.72	kJ/mol	Joback Method
hf	-670.01	kJ/mol	Joback Method
hfus	48.35	kJ/mol	Joback Method
hvap	73.89	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.346		Crippen Method
mcvol	270.760	ml/mol	McGowan Method
pc	1322.31	kPa	Joback Method
rinpol	2187.00		NIST Webbook
rinpol	2187.00		NIST Webbook
tb	772.14	K	Joback Method
tc	958.03	K	Joback Method
tf	426.78	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	800.69	J/mol×K	772.14	Joback Method
cpg	817.04	J/mol×K	803.12	Joback Method
cpg	832.51	J/mol×K	834.10	Joback Method
cpg	847.15	J/mol×K	865.08	Joback Method
cpg	860.98	J/mol×K	896.06	Joback Method
cpg	874.02	J/mol×K	927.05	Joback Method
cpg	886.32	J/mol×K	958.03	Joback Method
dvisc	0.0008949	Pa×s	426.78	Joback Method

dvisc	0.0004226	Pa×s	484.34	Joback Method
dvisc	0.0002341	Pa×s	541.90	Joback Method
dvisc	0.0001452	Pa×s	599.46	Joback Method
dvisc	0.0000979	Pa×s	657.02	Joback Method
dvisc	0.0000704	Pa×s	714.58	Joback Method
dvisc	0.0000531	Pa×s	772.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348864&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