Fumaric acid, 2-hexyl octyl ester

Inchi: InChI=1S/C18H32O4/c1-4-6-8-9-10-11-15-21-17(19)13-14-18(20)22-16(3)12-7-5-2/h13-1
InchiKey: WMPJPFTWMSHGIR-BUHFOSPRSA-N
Formula: C18H32O4
SMILES: CCCCCCCCOC(=O)C=CC(=O)OC(C)CCCC
Mol. weight [g/mol]: 312.44

Physical Properties

Property code	Value	Unit	Source
gf	-289.38	kJ/mol	Joback Method
hf	-792.51	kJ/mol	Joback Method
hfus	44.63	kJ/mol	Joback Method
hvap	73.54	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.568		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
pc	1280.99	kPa	Joback Method
rinpol	2106.00		NIST Webbook
tb	767.54	K	Joback Method
tc	951.19	K	Joback Method
tf	416.86	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.70	J/mol×K	767.54	Joback Method
cpg	842.72	J/mol×K	798.15	Joback Method
cpg	858.83	J/mol×K	828.76	Joback Method
cpg	874.04	J/mol×K	859.37	Joback Method
cpg	888.37	J/mol×K	889.97	Joback Method
cpg	901.84	J/mol×K	920.58	Joback Method
cpg	914.48	J/mol×K	951.19	Joback Method
dvisc	0.0011565	Pa×s	416.86	Joback Method
dvisc	0.0005130	Pa×s	475.31	Joback Method

dvisc	0.0002719	Pa×s	533.75	Joback Method
dvisc	0.0001633	Pa×s	592.20	Joback Method
dvisc	0.0001075	Pa×s	650.65	Joback Method
dvisc	0.0000758	Pa×s	709.09	Joback Method
dvisc	0.0000564	Pa×s	767.54	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=U348746&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