Fumaric acid, octyl pent-4-enyl ester

Inchi: InChI=1S/C17H28O4/c1-3-5-7-8-9-11-15-21-17(19)13-12-16(18)20-14-10-6-4-2/h4,12-13
InchiKey: KBNAFOHVDNHYOS-OUKQBFOZSA-N
Formula: C17H28O4
SMILES: C=CCCCOC(=O)C=CC(=O)OCCCCCCCC
Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-207.52	kJ/mol	Joback Method
hf	-641.16	kJ/mol	Joback Method
hfus	44.28	kJ/mol	Joback Method
hvap	71.04	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.956		Crippen Method
mcvol	256.670	ml/mol	McGowan Method
pc	1409.07	kPa	Joback Method
rinpol	2087.00		NIST Webbook
tb	741.78	K	Joback Method
tc	924.39	K	Joback Method
tf	418.83	K	Joback Method
vc	0.997	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.08	J/mol×K	741.78	Joback Method
cpg	813.67	J/mol×K	893.95	Joback Method
cpg	800.94	J/mol×K	863.52	Joback Method
cpg	787.43	J/mol×K	833.08	Joback Method
cpg	773.14	J/mol×K	802.65	Joback Method
cpg	758.03	J/mol×K	772.21	Joback Method
cpg	825.65	J/mol×K	924.39	Joback Method
dvisc	0.0000744	Pa×s	741.78	Joback Method
dvisc	0.0000974	Pa×s	687.95	Joback Method

dvisc	0.0001335	Pa×s	634.13	Joback Method
dvisc	0.0001942	Pa×s	580.30	Joback Method
dvisc	0.0003047	Pa×s	526.48	Joback Method
dvisc	0.0005300	Pa×s	472.65	Joback Method
dvisc	0.0010628	Pa×s	418.83	Joback Method

Sources

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=U348850&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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