Fumaric acid, octyl pent-4-en-2-yl ester

Inchi: InChI=1S/C17H28O4/c1-4-6-7-8-9-10-14-20-16(18)12-13-17(19)21-15(3)11-5-2/h5,12-13
InchiKey: UHWGIXWBHFFSQP-OUKQBFOZSA-N
Formula: C17H28O4
SMILES: C=CCC(C)OC(=O)C=CC(=O)OCCCCCCCC
Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-209.96	kJ/mol	Joback Method
hf	-646.44	kJ/mol	Joback Method
hfus	40.76	kJ/mol	Joback Method
hvap	70.65	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	3.954		Crippen Method
mcvol	256.670	ml/mol	McGowan Method
pc	1417.57	kPa	Joback Method
rinpol	2000.00		NIST Webbook
rinpol	2000.00		NIST Webbook
tb	741.34	K	Joback Method
tc	925.92	K	Joback Method
tf	403.83	K	Joback Method
vc	0.991	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.59	J/mol×K	741.34	Joback Method
cpg	814.85	J/mol×K	895.16	Joback Method
cpg	802.03	J/mol×K	864.39	Joback Method
cpg	788.42	J/mol×K	833.63	Joback Method
cpg	773.99	J/mol×K	802.87	Joback Method
cpg	758.72	J/mol×K	772.10	Joback Method
cpg	826.89	J/mol×K	925.92	Joback Method
dvisc	0.0000686	Pa×s	741.34	Joback Method

dvisc	0.0000914	Pa×s	685.09	Joback Method
dvisc	0.0001283	Pa×s	628.84	Joback Method
dvisc	0.0001925	Pa×s	572.58	Joback Method
dvisc	0.0003155	Pa×s	516.33	Joback Method
dvisc	0.0005835	Pa×s	460.08	Joback Method
dvisc	0.0012808	Pa×s	403.83	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=U348927&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