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

Inchi: InChI=1S/C15H24O4/c1-3-5-7-9-13-19-15(17)11-10-14(16)18-12-8-6-4-2/h5,7,10-11H,3-
InchiKey: TXYAUZAXQBGEJS-WTQQXEBVSA-N
Formula: C15H24O4
SMILES: CCC=CCCOC(=O)C=CC(=O)OCCCCC
Mol. weight [g/mol]: 268.35

Physical Properties

Property code	Value	Unit	Source
gf	-231.98	kJ/mol	Joback Method
hf	-608.09	kJ/mol	Joback Method
hfus	40.58	kJ/mol	Joback Method
hvap	67.21	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.175		Crippen Method
mcvol	228.490	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
rinpol	1881.00		NIST Webbook
tb	703.50	K	Joback Method
tc	889.44	K	Joback Method
tf	392.97	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.78	J/mol×K	703.50	Joback Method
cpg	646.90	J/mol×K	734.49	Joback Method
cpg	661.24	J/mol×K	765.48	Joback Method
cpg	674.82	J/mol×K	796.47	Joback Method
cpg	687.68	J/mol×K	827.46	Joback Method
cpg	699.84	J/mol×K	858.45	Joback Method
cpg	711.31	J/mol×K	889.44	Joback Method
dvisc	0.0011790	Pa×s	392.97	Joback Method
dvisc	0.0005772	Pa×s	444.73	Joback Method

dvisc	0.0003279	Pa×s	496.48	Joback Method
dvisc	0.0002073	Pa×s	548.24	Joback Method
dvisc	0.0001418	Pa×s	599.99	Joback Method
dvisc	0.0001031	Pa×s	651.75	Joback Method
dvisc	0.0000785	Pa×s	703.50	Joback Method

Sources

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=U348886&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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