Fumaric acid, hexyl pent-4-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/h4,10-11H,2-3,
InchiKey: NYCIKEPAHUNUNQ-ZHACJKMWSA-N
Formula: C15H24O4
SMILES: C=CCCCOC(=O)C=CC(=O)OCCCCCC
Mol. weight [g/mol]: 268.35

Physical Properties

Property code	Value	Unit	Source
gf	-224.36	kJ/mol	Joback Method
hf	-599.88	kJ/mol	Joback Method
hfus	39.10	kJ/mol	Joback Method
hvap	66.58	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.175		Crippen Method
mcvol	228.490	ml/mol	McGowan Method
pc	1636.45	kPa	Joback Method
rinpol	1889.00		NIST Webbook
rinpol	1889.00		NIST Webbook
tb	696.02	K	Joback Method
tc	878.85	K	Joback Method
tf	396.29	K	Joback Method
vc	0.884	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.74	J/mol×K	696.02	Joback Method
cpg	698.72	J/mol×K	848.38	Joback Method
cpg	686.58	J/mol×K	817.91	Joback Method
cpg	673.73	J/mol×K	787.43	Joback Method
cpg	660.15	J/mol×K	756.96	Joback Method
cpg	645.83	J/mol×K	726.49	Joback Method
cpg	710.16	J/mol×K	878.85	Joback Method
dvisc	0.0000959	Pa×s	696.02	Joback Method

dvisc	0.0001248	Pa×s	646.06	Joback Method
dvisc	0.0001698	Pa×s	596.11	Joback Method
dvisc	0.0002442	Pa×s	546.15	Joback Method
dvisc	0.0003781	Pa×s	496.20	Joback Method
dvisc	0.0006454	Pa×s	446.25	Joback Method
dvisc	0.0012608	Pa×s	396.29	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=U348848&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