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

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

Physical Properties

Property code	Value	Unit	Source
gf	-229.24	kJ/mol	Joback Method
hf	-610.44	kJ/mol	Joback Method
hfus	32.06	kJ/mol	Joback Method
hvap	65.81	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.030		Crippen Method
mcvol	228.490	ml/mol	McGowan Method
pc	1657.84	kPa	Joback Method
rinpol	1755.00		NIST Webbook
rinpol	1755.00		NIST Webbook
tb	695.14	K	Joback Method
tc	883.11	K	Joback Method
tf	366.29	K	Joback Method
vc	0.873	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.73	J/mol×K	695.14	Joback Method
cpg	647.29	J/mol×K	726.47	Joback Method
cpg	662.03	J/mol×K	757.80	Joback Method
cpg	675.96	J/mol×K	789.12	Joback Method
cpg	689.11	J/mol×K	820.45	Joback Method
cpg	701.49	J/mol×K	851.78	Joback Method
cpg	713.12	J/mol×K	883.11	Joback Method
dvisc	0.0019351	Pa×s	366.29	Joback Method

dvisc	0.0008114	Pa×s	421.10	Joback Method
dvisc	0.0004156	Pa×s	475.91	Joback Method
dvisc	0.0002444	Pa×s	530.72	Joback Method
dvisc	0.0001588	Pa×s	585.52	Joback Method
dvisc	0.0001110	Pa×s	640.33	Joback Method
dvisc	0.0000822	Pa×s	695.14	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=U348925&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