

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

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

Physical Properties

Property code	Value	Unit	Source
gf	-226.80	kJ/mol	Joback Method
hf	-605.16	kJ/mol	Joback Method
hfus	35.58	kJ/mol	Joback Method
hvap	66.20	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.174		Crippen Method
mcvol	228.490	ml/mol	McGowan Method
pc	1647.09	kPa	Joback Method
rinqol	1799.00		NIST Webbook
tb	695.58	K	Joback Method
tc	880.91	K	Joback Method
tf	381.29	K	Joback Method
vc	0.878	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.23	J/molxK	695.58	Joback Method
cpg	646.56	J/molxK	726.47	Joback Method
cpg	661.08	J/molxK	757.36	Joback Method
cpg	674.83	J/molxK	788.25	Joback Method
cpg	687.83	J/molxK	819.13	Joback Method
cpg	700.08	J/molxK	850.02	Joback Method
cpg	711.62	J/molxK	880.91	Joback Method
dvisc	0.0015407	Paxs	381.29	Joback Method
dvisc	0.0007184	Paxs	433.67	Joback Method

dvisc	0.0003949	Paxs	486.05	Joback Method
dvisc	0.0002439	Paxs	538.44	Joback Method
dvisc	0.0001640	Paxs	590.82	Joback Method
dvisc	0.0001177	Paxs	643.20	Joback Method
dvisc	0.0000888	Paxs	695.58	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=U348926&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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