

Fumaric acid, cis-hex-3-enyl pentyl 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-OLCNXZRBSA-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
rinpola	1885.00		NIST Webbook
tb	703.50	K	Joback Method
tc	889.44	K	Joback Method
tf	392.97	K	Joback Method
vc	0.883	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0003279	Paxs	496.48	Joback Method
dvisc	0.0002073	Paxs	548.24	Joback Method
dvisc	0.0001418	Paxs	599.99	Joback Method
dvisc	0.0001031	Paxs	651.75	Joback Method
dvisc	0.0000785	Paxs	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=U348862&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

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