

Fumaric acid, cis-non-3-enyl hexyl ester

Inchi:	InChI=1S/C19H32O4/c1-3-5-7-9-10-11-13-17-23-19(21)15-14-18(20)22-16-12-8-6-4-2/h
InchiKey:	BAQJAYQDZOWVIE-HHAKQIEWSA-N
Formula:	C19H32O4
SMILES:	CCCCCC=CCCOC(=O)C=CC(=O)OCCCCC
Mol. weight [g/mol]:	324.45

Physical Properties

Property code	Value	Unit	Source
gf	-198.30	kJ/mol	Joback Method
hf	-690.65	kJ/mol	Joback Method
hfus	50.94	kJ/mol	Joback Method
hvap	76.12	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.736		Crippen Method
mcvol	284.850	ml/mol	McGowan Method
pc	1234.61	kPa	Joback Method
rinqol	2273.00		NIST Webbook
tb	795.02	K	Joback Method
tc	982.06	K	Joback Method
tf	438.05	K	Joback Method
vc	1.107	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	859.06	J/molxK	795.02	Joback Method
cpg	934.02	J/molxK	950.88	Joback Method
cpg	920.71	J/molxK	919.71	Joback Method
cpg	906.59	J/molxK	888.54	Joback Method
cpg	891.63	J/molxK	857.37	Joback Method
cpg	875.80	J/molxK	826.19	Joback Method
cpg	946.55	J/molxK	982.06	Joback Method
dvisc	0.0000463	Paxs	795.02	Joback Method
dvisc	0.0000616	Paxs	735.52	Joback Method

dvisc	0.0000859	Paxs	676.03	Joback Method
dvisc	0.0001279	Paxs	616.53	Joback Method
dvisc	0.0002074	Paxs	557.04	Joback Method
dvisc	0.0003774	Paxs	497.55	Joback Method
dvisc	0.0008079	Paxs	438.05	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=U348881&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

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