

Fumaric acid, di(cis-hex-3-enyl) ester

Other names:	(Z)-Hexenyl fumarate
Inchi:	InChI=1S/C16H24O4/c1-3-5-7-9-13-19-15(17)11-12-16(18)20-14-10-8-6-4-2/h5-8,11-12H
InchiKey:	QGNBTOILRVTESN-XGNN SBLXSA-N
Formula:	C16H24O4
SMILES:	CCC=CCCOC(=O)C=CC(=O)OCCC=CCC
Mol. weight [g/mol]:	280.36

Physical Properties

Property code	Value	Unit	Source
gf	-143.34	kJ/mol	Joback Method
hf	-511.51	kJ/mol	Joback Method
hfus	43.38	kJ/mol	Joback Method
hvap	69.40	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.342		Crippen Method
mvol	238.280	ml/mol	McGowan Method
pc	1592.35	kPa	Joback Method
tb	730.54	K	Joback Method
tc	921.10	K	Joback Method
tf	399.16	K	Joback Method
vc	0.919	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.30	J/molxK	730.54	Joback Method
cpg	678.33	J/molxK	762.30	Joback Method
cpg	692.57	J/molxK	794.06	Joback Method
cpg	706.05	J/molxK	825.82	Joback Method
cpg	718.80	J/molxK	857.58	Joback Method
cpg	730.86	J/molxK	889.34	Joback Method
cpg	742.28	J/molxK	921.10	Joback Method
dvisc	0.0010046	Paxs	399.16	Joback Method
dvisc	0.0004718	Paxs	454.39	Joback Method

dvisc	0.0002610	Paxs	509.62	Joback Method
dvisc	0.0001621	Paxs	564.85	Joback Method
dvisc	0.0001096	Paxs	620.08	Joback Method
dvisc	0.0000790	Paxs	675.31	Joback Method
dvisc	0.0000598	Paxs	730.54	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=U348876&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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