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

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-UXJRKJCUSA-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
mcvol	238.280	ml/mol	McGowan Method
pc	1592.35	kPa	Joback Method
rinpol	1985.00		NIST Webbook
tb	730.54	K	Joback Method
tc	921.10	K	Joback Method
tf	399.16	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.30	J/mol×K	730.54	Joback Method
cpg	730.86	J/mol×K	889.34	Joback Method
cpg	718.80	J/mol×K	857.58	Joback Method
cpg	706.05	J/mol×K	825.82	Joback Method
cpg	692.57	J/mol×K	794.06	Joback Method
cpg	678.33	J/mol×K	762.30	Joback Method
cpg	742.28	J/mol×K	921.10	Joback Method
dvisc	0.0000598	Pa×s	730.54	Joback Method
dvisc	0.0000790	Pa×s	675.31	Joback Method

dvisc	0.0001096	Pa×s	620.08	Joback Method
dvisc	0.0001621	Pa×s	564.85	Joback Method
dvisc	0.0002610	Pa×s	509.62	Joback Method
dvisc	0.0004718	Pa×s	454.39	Joback Method
dvisc	0.0010046	Pa×s	399.16	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=U348900&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