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

Inchi: InChI=1S/C19H32O4/c1-4-5-6-7-8-9-10-15-22-18(20)13-14-19(21)23-16-11-12-17(2)3/h8
InchiKey: IUACXUGKLOXHDY-NRSBDZSJSA-N
Formula: C19H32O4
SMILES: CCCCCC=CCCOC(=O)C=CC(=O)OCCCC(C)C
Mol. weight [g/mol]: 324.45

Physical Properties

Property code	Value	Unit	Source
gf	-200.74	kJ/mol	Joback Method
hf	-695.93	kJ/mol	Joback Method
hfus	47.42	kJ/mol	Joback Method
hvap	75.73	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.592		Crippen Method
mcvol	284.850	ml/mol	McGowan Method
pc	1241.58	kPa	Joback Method
rinpol	2226.00		NIST Webbook
rinpol	2226.00		NIST Webbook
tb	794.58	K	Joback Method
tc	983.09	K	Joback Method
tf	423.05	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	859.57	J/mol×K	794.58	Joback Method
cpg	876.44	J/mol×K	826.00	Joback Method
cpg	892.38	J/mol×K	857.42	Joback Method
cpg	907.43	J/mol×K	888.83	Joback Method
cpg	921.61	J/mol×K	920.25	Joback Method
cpg	934.97	J/mol×K	951.67	Joback Method
cpg	947.53	J/mol×K	983.09	Joback Method
dvisc	0.0009683	Pa×s	423.05	Joback Method

dvisc	0.0004126	Pa×s	484.97	Joback Method
dvisc	0.0002133	Pa×s	546.89	Joback Method
dvisc	0.0001261	Pa×s	608.82	Joback Method
dvisc	0.0000821	Pa×s	670.74	Joback Method
dvisc	0.0000575	Pa×s	732.66	Joback Method
dvisc	0.0000426	Pa×s	794.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348880&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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