Fumaric acid, isohexyl trans-hex-3-enyl ester

Inchi: InChI=1S/C16H26O4/c1-4-5-6-7-12-19-15(17)10-11-16(18)20-13-8-9-14(2)3/h5-6,10-11,
InchiKey: MRRWQERSRCFCQB-RINXSNKBSA-N
Formula: C16H26O4
SMILES: CCC=CCCOC(=O)C=CC(=O)OCCCC(C)C
Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
gf	-226.00	kJ/mol	Joback Method
hf	-634.01	kJ/mol	Joback Method
hfus	39.65	kJ/mol	Joback Method
hvap	69.05	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.421		Crippen Method
mcvol	242.580	ml/mol	McGowan Method
pc	1537.87	kPa	Joback Method
rinpol	1940.00		NIST Webbook
rinpol	1940.00		NIST Webbook
tb	725.94	K	Joback Method
tc	913.65	K	Joback Method
tf	389.24	K	Joback Method
vc	0.933	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	687.48	J/mol×K	725.94	Joback Method
cpg	758.20	J/mol×K	882.37	Joback Method
cpg	745.62	J/mol×K	851.08	Joback Method
cpg	732.28	J/mol×K	819.80	Joback Method
cpg	718.17	J/mol×K	788.51	Joback Method
cpg	703.24	J/mol×K	757.23	Joback Method
cpg	770.05	J/mol×K	913.65	Joback Method
dvisc	0.0000639	Pa×s	725.94	Joback Method

dvisc	0.0000857	Pa×s	669.82	Joback Method
dvisc	0.0001212	Pa×s	613.71	Joback Method
dvisc	0.0001840	Pa×s	557.59	Joback Method
dvisc	0.0003066	Pa×s	501.47	Joback Method
dvisc	0.0005810	Pa×s	445.36	Joback Method
dvisc	0.0013237	Pa×s	389.24	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=U348887&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