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

Inchi: InChI=1S/C13H20O4/c1-3-5-6-7-11-17-13(15)9-8-12(14)16-10-4-2/h5-6,8-9H,3-4,7,10-11
InchiKey: SSGOPRWMTHYQSV-HHWLVVFRSA-N
Formula: C13H20O4
SMILES: CCC=CCCOC(=O)C=CC(=O)OCCC
Mol. weight [g/mol]: 240.30

Physical Properties

Property code	Value	Unit	Source
gf	-248.82	kJ/mol	Joback Method
hf	-566.81	kJ/mol	Joback Method
hfus	35.40	kJ/mol	Joback Method
hvap	62.76	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.395		Crippen Method
mcvol	200.310	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	1676.00		NIST Webbook
tb	657.74	K	Joback Method
tc	846.12	K	Joback Method
tf	370.43	K	Joback Method
vc	0.771	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.14	J/mol×K	657.74	Joback Method
cpg	539.27	J/mol×K	689.14	Joback Method
cpg	552.69	J/mol×K	720.53	Joback Method
cpg	565.41	J/mol×K	751.93	Joback Method
cpg	577.46	J/mol×K	783.32	Joback Method
cpg	588.85	J/mol×K	814.72	Joback Method
cpg	599.61	J/mol×K	846.12	Joback Method
dvisc	0.0013734	Pa×s	370.43	Joback Method
dvisc	0.0006908	Pa×s	418.31	Joback Method

dvisc	0.0004002	Pa×s	466.20	Joback Method
dvisc	0.0002566	Pa×s	514.09	Joback Method
dvisc	0.0001775	Pa×s	561.97	Joback Method
dvisc	0.0001301	Pa×s	609.86	Joback Method
dvisc	0.0000998	Pa×s	657.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348883&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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