Fumaric acid, dec-4-enyl isobutyl ester

Inchi: InChI=1S/C18H30O4/c1-4-5-6-7-8-9-10-11-14-21-17(19)12-13-18(20)22-15-16(2)3/h8-9,
InchiKey: ICXRNQIODIVYQE-AFAJWACHSA-N
Formula: C18H30O4
SMILES: CCCCCC=CCCCOC(=O)C=CC(=O)OCC(C)C
Mol. weight [g/mol]: 310.43

Physical Properties

Property code	Value	Unit	Source
gf	-209.16	kJ/mol	Joback Method
hf	-675.29	kJ/mol	Joback Method
hfus	44.83	kJ/mol	Joback Method
hvap	73.50	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.202		Crippen Method
mcvol	270.760	ml/mol	McGowan Method
pc	1330.04	kPa	Joback Method
rinpol	2121.00		NIST Webbook
rinpol	2121.00		NIST Webbook
tb	771.70	K	Joback Method
tc	959.35	K	Joback Method
tf	411.78	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	801.20	J/mol×K	771.70	Joback Method
cpg	875.10	J/mol×K	928.08	Joback Method
cpg	861.99	J/mol×K	896.80	Joback Method
cpg	848.07	J/mol×K	865.53	Joback Method
cpg	833.33	J/mol×K	834.25	Joback Method
cpg	817.71	J/mol×K	802.98	Joback Method
cpg	887.44	J/mol×K	959.35	Joback Method
dvisc	0.0000489	Pa×s	771.70	Joback Method

dvisc	0.0000659	Pa×s	711.71	Joback Method
dvisc	0.0000939	Pa×s	651.73	Joback Method
dvisc	0.0001435	Pa×s	591.74	Joback Method
dvisc	0.0002417	Pa×s	531.75	Joback Method
dvisc	0.0004645	Pa×s	471.77	Joback Method
dvisc	0.0010798	Pa×s	411.78	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348937&Units=SI

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