Fumaric acid, isobutyl pent-4-enyl ester

Inchi: InChI=1S/C13H20O4/c1-4-5-6-9-16-12(14)7-8-13(15)17-10-11(2)3/h4,7-8,11H,1,5-6,9-10
InchiKey: HHXQOEXPOISSEC-BQYQJAHWSA-N
Formula: C13H20O4
SMILES: C=CCCCOC(=O)C=CC(=O)OCC(C)C
Mol. weight [g/mol]: 240.30

Physical Properties

Property code	Value	Unit	Source
gf	-243.64	kJ/mol	Joback Method
hf	-563.88	kJ/mol	Joback Method
hfus	30.40	kJ/mol	Joback Method
hvap	61.74	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.251		Crippen Method
mcvol	200.310	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
rinpol	1627.00		NIST Webbook
rinpol	1627.00		NIST Webbook
tb	649.82	K	Joback Method
tc	837.70	K	Joback Method
tf	358.75	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.80	J/mol×K	649.82	Joback Method
cpg	539.15	J/mol×K	681.13	Joback Method
cpg	552.77	J/mol×K	712.45	Joback Method
cpg	565.68	J/mol×K	743.76	Joback Method
cpg	577.90	J/mol×K	775.07	Joback Method
cpg	589.43	J/mol×K	806.39	Joback Method
cpg	600.30	J/mol×K	837.70	Joback Method
dvisc	0.0018071	Pa×s	358.75	Joback Method

dvisc	0.0008647	Pa×s	407.26	Joback Method
dvisc	0.0004841	Pa×s	455.77	Joback Method
dvisc	0.0003030	Pa×s	504.28	Joback Method
dvisc	0.0002059	Pa×s	552.80	Joback Method
dvisc	0.0001489	Pa×s	601.31	Joback Method
dvisc	0.0001130	Pa×s	649.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348846&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