Fumaric acid, butyl pent-4-enyl ester

Inchi: InChI=1S/C13H20O4/c1-3-5-7-11-17-13(15)9-8-12(14)16-10-6-4-2/h3,8-9H,1,4-7,10-11H
InchiKey: UPWPLXAPKLFNSX-CMDGGOBGSA-N
Formula: C13H20O4
SMILES: C=CCCCOC(=O)C=CC(=O)OCCCC
Mol. weight [g/mol]: 240.30

Physical Properties

Property code	Value	Unit	Source
gf	-241.20	kJ/mol	Joback Method
hf	-558.60	kJ/mol	Joback Method
hfus	33.92	kJ/mol	Joback Method
hvap	62.13	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.395		Crippen Method
mcvol	200.310	ml/mol	McGowan Method
pc	1923.67	kPa	Joback Method
rinpol	1679.00		NIST Webbook
tb	650.26	K	Joback Method
tc	835.14	K	Joback Method
tf	373.75	K	Joback Method
vc	0.772	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.33	J/mol×K	650.26	Joback Method
cpg	538.41	J/mol×K	681.07	Joback Method
cpg	551.80	J/mol×K	711.89	Joback Method
cpg	564.51	J/mol×K	742.70	Joback Method
cpg	576.55	J/mol×K	773.51	Joback Method
cpg	587.94	J/mol×K	804.33	Joback Method
cpg	598.69	J/mol×K	835.14	Joback Method
dvisc	0.0014567	Pa×s	373.75	Joback Method
dvisc	0.0007674	Pa×s	419.83	Joback Method

dvisc	0.0004590	Pa×s	465.92	Joback Method
dvisc	0.0003011	Pa×s	512.00	Joback Method
dvisc	0.0002118	Pa×s	558.09	Joback Method
dvisc	0.0001571	Pa×s	604.17	Joback Method
dvisc	0.0001217	Pa×s	650.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348847&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