Fumaric acid, 2-methylpent-3-yl propyl ester

Inchi: InChI=1S/C13H22O4/c1-5-9-16-12(14)7-8-13(15)17-11(6-2)10(3)4/h7-8,10-11H,5-6,9H2,
InchiKey: RUIRBMCGUFVVHS-BQYQJAHWSA-N
Formula: C13H22O4
SMILES: CCCOC(=O)C=CC(=O)OC(CC)C(C)C
Mol. weight [g/mol]: 242.31

Physical Properties

Property code	Value	Unit	Source
gf	-333.92	kJ/mol	Joback Method
hf	-694.59	kJ/mol	Joback Method
hfus	28.16	kJ/mol	Joback Method
hvap	62.03	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.474		Crippen Method
mcvol	204.610	ml/mol	McGowan Method
pc	1880.53	kPa	Joback Method
rinpol	1566.00		NIST Webbook
rinpol	1566.00		NIST Webbook
tb	652.70	K	Joback Method
tc	840.76	K	Joback Method
tf	345.51	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.81	J/mol×K	652.70	Joback Method
cpg	562.99	J/mol×K	684.04	Joback Method
cpg	577.41	J/mol×K	715.39	Joback Method
cpg	591.08	J/mol×K	746.73	Joback Method
cpg	604.02	J/mol×K	778.07	Joback Method
cpg	616.23	J/mol×K	809.41	Joback Method
cpg	627.73	J/mol×K	840.76	Joback Method
dvisc	0.0023733	Pa×s	345.51	Joback Method

dvisc	0.0009966	Pa×s	396.71	Joback Method
dvisc	0.0005103	Pa×s	447.91	Joback Method
dvisc	0.0002998	Pa×s	499.11	Joback Method
dvisc	0.0001944	Pa×s	550.30	Joback Method
dvisc	0.0001357	Pa×s	601.50	Joback Method
dvisc	0.0001003	Pa×s	652.70	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=U348759&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