Fumaric acid, pent-4-en-2-yl pentyl ester

Inchi: InChI=1S/C14H22O4/c1-4-6-7-11-17-13(15)9-10-14(16)18-12(3)8-5-2/h5,9-10,12H,2,4,6-
InchiKey: YABBSNQIOLRGCJ-MDZDMXLPSA-N
Formula: C14H22O4
SMILES: C=CCC(C)OC(=O)C=CC(=O)OCCCCC
Mol. weight [g/mol]: 254.32

Physical Properties

Property code	Value	Unit	Source
gf	-235.22	kJ/mol	Joback Method
hf	-584.52	kJ/mol	Joback Method
hfus	32.99	kJ/mol	Joback Method
hvap	63.97	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.784		Crippen Method
mcvol	214.400	ml/mol	McGowan Method
pc	1783.35	kPa	Joback Method
rinpol	1705.00		NIST Webbook
tb	672.70	K	Joback Method
tc	859.11	K	Joback Method
tf	370.02	K	Joback Method
vc	0.823	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.36	J/mol×K	672.70	Joback Method
cpg	592.22	J/mol×K	703.77	Joback Method
cpg	606.32	J/mol×K	734.84	Joback Method
cpg	619.68	J/mol×K	765.90	Joback Method
cpg	632.31	J/mol×K	796.97	Joback Method
cpg	644.22	J/mol×K	828.04	Joback Method
cpg	655.45	J/mol×K	859.11	Joback Method
dvisc	0.0016744	Pa×s	370.02	Joback Method
dvisc	0.0007907	Pa×s	420.47	Joback Method

dvisc	0.0004385	Pa×s	470.91	Joback Method
dvisc	0.0002725	Pa×s	521.36	Joback Method
dvisc	0.0001842	Pa×s	571.81	Joback Method
dvisc	0.0001327	Pa×s	622.25	Joback Method
dvisc	0.0001004	Pa×s	672.70	Joback Method

Sources

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=U348924&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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