

Fumaric acid, di(pent-4-en-2-yl) ester

Inchi:

lnchl=1S/C14H20O4/c1-5-7-11(3)17-13(15)9-10-14(16)18-12(4)8-6-2/h5-6,9-12H,1-2,7-8

InchiKey:

ONSTWLLKVJJSQB-MDZDMXLPSA-N

Formula:

C14H20O4

SMILES:

C=CCC(C)OC(=O)C=CC(=O)OC(C)CC=C

Mol. weight [g/mol]:

252.31

Physical Properties

Property code	Value	Unit	Source
gf	-149.82	kJ/mol	Joback Method
hf	-464.37	kJ/mol	Joback Method
hfus	28.19	kJ/mol	Joback Method
hvap	62.91	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	2.558		Crippen Method
mcvol	210.100	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	1616.00		NIST Webbook
tb	668.94	K	Joback Method
tc	861.10	K	Joback Method
tf	353.26	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	554.78	J/mol×K	668.94	Joback Method
cpg	569.35	J/mol×K	700.97	Joback Method
cpg	583.13	J/mol×K	732.99	Joback Method
cpg	596.14	J/mol×K	765.02	Joback Method
cpg	608.40	J/mol×K	797.04	Joback Method
cpg	619.94	J/mol×K	829.07	Joback Method
cpg	630.77	J/mol×K	861.10	Joback Method
dvisc	0.0020747	Pa×s	353.26	Joback Method
dvisc	0.0008964	Pa×s	405.87	Joback Method

dvisc	0.0004696	Pa×s	458.49	Joback Method
dvisc	0.0002810	Pa×s	511.10	Joback Method
dvisc	0.0001851	Pa×s	563.71	Joback Method
dvisc	0.0001309	Pa×s	616.33	Joback Method
dvisc	0.0000978	Pa×s	668.94	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=U348934&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

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