

Fumaric acid, di(pent-4-enyl) ester

Inchi:

InChI=1S/C14H20O4/c1-3-5-7-11-17-13(15)9-10-14(16)18-12-8-6-4-2/h3-4,9-10H,1-2,5-8H

InchiKey:

AUCLTYLEVXSTDN-MDZDMXLPSA-N

Formula:

C14H20O4

SMILES:

C=CCCCOC(=O)C=CC(=O)OCCCC=C

Mol. weight [g/mol]:

252.31

Physical Properties

Property code	Value	Unit	Source
gf	-144.94	kJ/mol	Joback Method
hf	-453.81	kJ/mol	Joback Method
hfus	35.23	kJ/mol	Joback Method
hvap	63.69	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.561		Crippen Method
mcvol	210.100	ml/mol	McGowan Method
pc	1835.69	kPa	Joback Method
rinpol	1807.00		NIST Webbook
rinpol	1807.00		NIST Webbook
tb	669.82	K	Joback Method
tc	856.03	K	Joback Method
tf	383.26	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.80	J/mol×K	669.82	Joback Method
cpg	617.02	J/mol×K	825.00	Joback Method
cpg	605.75	J/mol×K	793.96	Joback Method
cpg	593.81	J/mol×K	762.93	Joback Method
cpg	581.19	J/mol×K	731.89	Joback Method
cpg	567.86	J/mol×K	700.86	Joback Method
cpg	627.65	J/mol×K	856.03	Joback Method
dvisc	0.0001137	Pa×s	669.82	Joback Method

dvisc	0.0001465	Pa×s	622.06	Joback Method
dvisc	0.0001968	Pa×s	574.30	Joback Method
dvisc	0.0002791	Pa×s	526.54	Joback Method
dvisc	0.0004243	Pa×s	478.78	Joback Method
dvisc	0.0007079	Pa×s	431.02	Joback Method
dvisc	0.0013415	Pa×s	383.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348858&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mccvol:	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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