

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

Inchi:	InChI=1S/C19H32O4/c1-4-6-7-8-9-10-11-12-16-22-18(20)14-15-19(21)23-17(3)13-5-2/h5
InchiKey:	GBLKVHIAAKBKTQ-CCEZHUSRSA-N
Formula:	C19H32O4
SMILES:	<chem>C=CCC(C)OC(=O)C=CC(=O)OCCCCCCCCC</chem>
Mol. weight [g/mol]:	324.45

Physical Properties

Property code	Value	Unit	Source
gf	-193.12	kJ/mol	Joback Method
hf	-687.72	kJ/mol	Joback Method
hfus	45.94	kJ/mol	Joback Method
hvap	75.10	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.734		Crippen Method
mvol	284.850	ml/mol	McGowan Method
pc	1232.88	kPa	Joback Method
rinpol	2191.00		NIST Webbook
rinpol	2191.00		NIST Webbook
tb	787.10	K	Joback Method
tc	973.13	K	Joback Method
tf	426.37	K	Joback Method
vc	1.103	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	858.20	J/molxK	787.10	Joback Method
cpg	875.08	J/molxK	818.11	Joback Method
cpg	891.01	J/molxK	849.11	Joback Method
cpg	906.03	J/molxK	880.12	Joback Method
cpg	920.17	J/molxK	911.12	Joback Method
cpg	933.45	J/molxK	942.13	Joback Method
cpg	945.90	J/molxK	973.13	Joback Method
dvisc	0.0010425	Paxs	426.37	Joback Method

dvisc	0.0004651	Paxs	486.49	Joback Method
dvisc	0.0002478	Paxs	546.61	Joback Method
dvisc	0.0001496	Paxs	606.73	Joback Method
dvisc	0.0000989	Paxs	666.86	Joback Method
dvisc	0.0000700	Paxs	726.98	Joback Method
dvisc	0.0000522	Paxs	787.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348929&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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