

Fumaric acid, 3-heptyl nonyl ester

Inchi:	InChI=1S/C20H36O4/c1-4-7-9-10-11-12-13-17-23-19(21)15-16-20(22)24-18(6-3)14-8-5-2
InchiKey:	VFOVRYXCNJSKMH-FOCLMDBBSA-N
Formula:	C20H36O4
SMILES:	CCCCCCCCCOC(=O)C=CC(=O)OC(CC)CCCC
Mol. weight [g/mol]:	340.50

Physical Properties

Property code	Value	Unit	Source
gf	-272.54	kJ/mol	Joback Method
hf	-833.79	kJ/mol	Joback Method
hfus	49.81	kJ/mol	Joback Method
hvap	78.00	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	5.348		Crippen Method
mcvol	303.240	ml/mol	McGowan Method
pc	1121.55	kPa	Joback Method
rinpol	2277.00		NIST Webbook
tb	813.30	K	Joback Method
tc	1000.35	K	Joback Method
tf	439.40	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	944.36	J/molxK	813.30	Joback Method
cpg	1023.32	J/molxK	969.18	Joback Method
cpg	1009.45	J/molxK	938.00	Joback Method
cpg	994.65	J/molxK	906.83	Joback Method
cpg	978.88	J/molxK	875.65	Joback Method
cpg	962.12	J/molxK	844.48	Joback Method
cpg	1036.28	J/molxK	1000.35	Joback Method
dvisc	0.0000425	Paxs	813.30	Joback Method
dvisc	0.0000574	Paxs	750.98	Joback Method

dvisc	0.0000819	Paxs	688.67	Joback Method
dvisc	0.0001253	Paxs	626.35	Joback Method
dvisc	0.0002106	Paxs	564.03	Joback Method
dvisc	0.0004027	Paxs	501.72	Joback Method
dvisc	0.0009257	Paxs	439.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348686&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
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
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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