

Fumaric acid, 8-chlorooctyl decyl ester

Inchi:	InChI=1S/C22H39ClO4/c1-2-3-4-5-6-8-11-14-19-26-21(24)16-17-22(25)27-20-15-12-9-7
InchiKey:	LZFVNKBKTMUJRA-WUKNDPDISA-N
Formula:	C22H39ClO4
SMILES:	CCCCCCCCCOC(=O)C=CC(=O)OCCCCCCCCCI
Mol. weight [g/mol]:	403.00

Physical Properties

Property code	Value	Unit	Source
gf	-265.19	kJ/mol	Joback Method
hf	-885.53	kJ/mol	Joback Method
hfus	62.71	kJ/mol	Joback Method
hvap	87.22	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	6.349		Crippen Method
mvol	343.660	ml/mol	McGowan Method
pc	962.67	kPa	Joback Method
rinpol	2928.00		NIST Webbook
rinpol	2928.00		NIST Webbook
tb	896.93	K	Joback Method
tc	1098.10	K	Joback Method
tf	506.86	K	Joback Method
vc	1.345	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1096.35	J/molxK	896.93	Joback Method
cpg	1114.04	J/molxK	930.46	Joback Method
cpg	1130.56	J/molxK	963.99	Joback Method
cpg	1145.96	J/molxK	997.51	Joback Method
cpg	1160.28	J/molxK	1031.04	Joback Method
cpg	1173.55	J/molxK	1064.57	Joback Method
cpg	1185.83	J/molxK	1098.10	Joback Method
dvisc	0.0004850	Paxs	506.86	Joback Method

dvisc	0.0002331	Paxs	571.87	Joback Method
dvisc	0.0001301	Paxs	636.88	Joback Method
dvisc	0.0000809	Paxs	701.89	Joback Method
dvisc	0.0000546	Paxs	766.91	Joback Method
dvisc	0.0000391	Paxs	831.92	Joback Method
dvisc	0.0000294	Paxs	896.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348537&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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