

Fumaric acid, cis-hex-3-enyl dodecyl ester

Inchi:	InChI=1S/C22H38O4/c1-3-5-7-9-10-11-12-13-14-16-20-26-22(24)18-17-21(23)25-19-15-
InchiKey:	KBZDUHZWYUFGIO-MFSOAIKKS-A-N
Formula:	C22H38O4
SMILES:	CCC=CCCOC(=O)C=CC(=O)OCCCCCCCCCCCC
Mol. weight [g/mol]:	366.53

Physical Properties

Property code	Value	Unit	Source
gf	-173.04	kJ/mol	Joback Method
hf	-752.57	kJ/mol	Joback Method
hfus	58.71	kJ/mol	Joback Method
hvap	82.79	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	5.906		Crippen Method
mcvol	327.120	ml/mol	McGowan Method
pc	1018.13	kPa	Joback Method
rinpola	2590.00		NIST Webbook
tb	863.66	K	Joback Method
tc	1058.41	K	Joback Method
tf	471.86	K	Joback Method
vc	1.276	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1039.41	J/molxK	863.66	Joback Method
cpg	1057.40	J/molxK	896.12	Joback Method
cpg	1074.36	J/molxK	928.58	Joback Method
cpg	1090.31	J/molxK	961.04	Joback Method
cpg	1105.31	J/molxK	993.50	Joback Method
cpg	1119.40	J/molxK	1025.96	Joback Method
cpg	1132.62	J/molxK	1058.41	Joback Method
dvisc	0.0005794	Paxs	471.86	Joback Method
dvisc	0.0002626	Paxs	537.16	Joback Method

dvisc	0.0001413	Paxs	602.46	Joback Method
dvisc	0.0000858	Paxs	667.76	Joback Method
dvisc	0.0000570	Paxs	733.06	Joback Method
dvisc	0.0000405	Paxs	798.36	Joback Method
dvisc	0.0000302	Paxs	863.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348867&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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