

Fumaric acid, 2-decyl undecyl ester

Inchi:	InChI=1S/C25H46O4/c1-4-6-8-10-12-13-14-16-18-22-28-24(26)20-21-25(27)29-23(3)19-
InchiKey:	XNCUGUCRNCETCV-QZQOTICOSA-N
Formula:	C25H46O4
SMILES:	CCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)CCCCCCCC
Mol. weight [g/mol]:	410.63

Physical Properties

Property code	Value	Unit	Source
gf	-230.44	kJ/mol	Joback Method
hf	-936.99	kJ/mol	Joback Method
hfus	62.76	kJ/mol	Joback Method
hvap	89.13	kJ/mol	Joback Method
log10ws	-7.98		Crippen Method
logp	7.299		Crippen Method
mvol	373.690	ml/mol	McGowan Method
pc	832.42	kPa	Joback Method
rinpol	2777.00		NIST Webbook
rinpol	2777.00		NIST Webbook
tb	927.70	K	Joback Method
tc	1137.27	K	Joback Method
tf	495.75	K	Joback Method
vc	1.458	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1254.19	J/molxK	927.70	Joback Method
cpg	1340.92	J/molxK	1102.34	Joback Method
cpg	1326.14	J/molxK	1067.41	Joback Method
cpg	1310.14	J/molxK	1032.49	Joback Method
cpg	1292.84	J/molxK	997.56	Joback Method
cpg	1274.21	J/molxK	962.63	Joback Method
cpg	1354.51	J/molxK	1137.27	Joback Method
dvisc	0.0000202	Paxs	927.70	Joback Method

dvisc	0.0000275	Paxs	855.71	Joback Method
dvisc	0.0000396	Paxs	783.72	Joback Method
dvisc	0.0000616	Paxs	711.72	Joback Method
dvisc	0.0001057	Paxs	639.73	Joback Method
dvisc	0.0002080	Paxs	567.74	Joback Method
dvisc	0.0004981	Paxs	495.75	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348592&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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