

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

Inchi: InChI=1S/C23H40O4/c1-4-6-7-8-9-10-11-12-13-14-15-16-20-26-22(24)18-19-23(25)27-2
InchiKey: VCUQKMACEJNVBR-VHEBQXMUSA-N
Formula: C23H40O4
SMILES: C=CCC(C)OC(=O)C=CC(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 380.56

Physical Properties

Property code	Value	Unit	Source
gf	-159.44	kJ/mol	Joback Method
hf	-770.28	kJ/mol	Joback Method
hfus	56.30	kJ/mol	Joback Method
hvap	84.00	kJ/mol	Joback Method
log10ws	-6.99		Crippen Method
logp	6.295		Crippen Method
mvol	341.210	ml/mol	McGowan Method
pc	957.32	kPa	Joback Method
rinpol	2595.00		NIST Webbook
rinpol	2595.00		NIST Webbook
tb	878.62	K	Joback Method
tc	1075.92	K	Joback Method
tf	471.45	K	Joback Method
vc	1.327	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1099.87	J/molxK	878.62	Joback Method
cpg	1118.33	J/molxK	911.50	Joback Method
cpg	1135.64	J/molxK	944.39	Joback Method
cpg	1151.84	J/molxK	977.27	Joback Method
cpg	1166.96	J/molxK	1010.16	Joback Method
cpg	1181.07	J/molxK	1043.04	Joback Method
cpg	1194.18	J/molxK	1075.92	Joback Method
dvisc	0.0006567	Paxs	471.45	Joback Method

dvisc	0.0002824	Paxs	539.31	Joback Method
dvisc	0.0001467	Paxs	607.17	Joback Method
dvisc	0.0000869	Paxs	675.03	Joback Method
dvisc	0.0000567	Paxs	742.90	Joback Method
dvisc	0.0000397	Paxs	810.76	Joback Method
dvisc	0.0000294	Paxs	878.62	Joback Method

Sources

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=U348933&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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