

Fumaric acid, pent-4-enyl tetradecyl ester

Inchi:	InChI=1S/C23H40O4/c1-3-5-7-8-9-10-11-12-13-14-15-17-21-27-23(25)19-18-22(24)26-2
InchiKey:	GWSDQTQHQSQCSK-VHEBQXMUSA-N
Formula:	C23H40O4
SMILES:	C=CCCCOC(=O)C=CC(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	380.56

Physical Properties

Property code	Value	Unit	Source
gf	-157.00	kJ/mol	Joback Method
hf	-765.00	kJ/mol	Joback Method
hfus	59.82	kJ/mol	Joback Method
hvap	84.39	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	6.296		Crippen Method
mcvol	341.210	ml/mol	McGowan Method
pc	952.60	kPa	Joback Method
rinpol	2681.00		NIST Webbook
tb	879.06	K	Joback Method
tc	1076.27	K	Joback Method
tf	486.45	K	Joback Method
vc	1.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1099.42	J/molxK	879.06	Joback Method
cpg	1117.89	J/molxK	911.93	Joback Method
cpg	1135.22	J/molxK	944.80	Joback Method
cpg	1151.44	J/molxK	977.67	Joback Method
cpg	1166.62	J/molxK	1010.53	Joback Method
cpg	1180.77	J/molxK	1043.40	Joback Method
cpg	1193.96	J/molxK	1076.27	Joback Method
dvisc	0.0005649	Paxs	486.45	Joback Method
dvisc	0.0002638	Paxs	551.88	Joback Method

dvisc	0.0001448	Paxs	617.32	Joback Method
dvisc	0.0000892	Paxs	682.76	Joback Method
dvisc	0.0000598	Paxs	748.19	Joback Method
dvisc	0.0000427	Paxs	813.62	Joback Method
dvisc	0.0000321	Paxs	879.06	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348854&Units=SI

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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