

Fumaric acid, trans-hex-3-enyl tridecyl ester

Inchi:	InChI=1S/C23H40O4/c1-3-5-7-9-10-11-12-13-14-15-17-21-27-23(25)19-18-22(24)26-20-
InchiKey:	NWYSCFQMVILLBL-OVWOTOAESA-N
Formula:	C23H40O4
SMILES:	CCC=CCCOC(=O)C=CC(=O)OCCCCCCCCCCCCC
Mol. weight [g/mol]:	380.56

Physical Properties

Property code	Value	Unit	Source
gf	-164.62	kJ/mol	Joback Method
hf	-773.21	kJ/mol	Joback Method
hfus	61.30	kJ/mol	Joback Method
hvap	85.02	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	6.296		Crippen Method
mcvol	341.210	ml/mol	McGowan Method
pc	958.51	kPa	Joback Method
rinsol	2676.00		NIST Webbook
tb	886.54	K	Joback Method
tc	1085.50	K	Joback Method
tf	483.13	K	Joback Method
vc	1.331	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1101.05	J/molxK	886.54	Joback Method
cpg	1119.53	J/molxK	919.70	Joback Method
cpg	1136.90	J/molxK	952.86	Joback Method
cpg	1153.22	J/molxK	986.02	Joback Method
cpg	1168.53	J/molxK	1019.18	Joback Method
cpg	1182.89	J/molxK	1052.34	Joback Method
cpg	1196.35	J/molxK	1085.50	Joback Method
dvisc	0.0005147	Paxs	483.13	Joback Method
dvisc	0.0002312	Paxs	550.37	Joback Method

dvisc	0.0001236	Paxs	617.60	Joback Method
dvisc	0.0000747	Paxs	684.84	Joback Method
dvisc	0.0000494	Paxs	752.07	Joback Method
dvisc	0.0000350	Paxs	819.31	Joback Method
dvisc	0.0000261	Paxs	886.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348893&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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