

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

Inchi:	InChI=1S/C24H42O4/c1-3-5-7-9-10-11-12-13-14-15-16-18-22-28-24(26)20-19-23(25)27-
InchiKey:	KKBXEHCLLYQXCD-CXIVGPKTSA-N
Formula:	C24H42O4
SMILES:	CCC=CCCOC(=O)C=CC(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	394.59

Physical Properties

Property code	Value	Unit	Source
gf	-156.20	kJ/mol	Joback Method
hf	-793.85	kJ/mol	Joback Method
hfus	63.89	kJ/mol	Joback Method
hvap	87.25	kJ/mol	Joback Method
log10ws	-7.30		Crippen Method
logp	6.686		Crippen Method
mcvol	355.300	ml/mol	McGowan Method
pc	903.97	kPa	Joback Method
rinsol	2767.00		NIST Webbook
tb	909.42	K	Joback Method
tc	1113.50	K	Joback Method
tf	494.40	K	Joback Method
vc	1.387	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1163.37	J/molxK	909.42	Joback Method
cpg	1182.36	J/molxK	943.43	Joback Method
cpg	1200.19	J/molxK	977.45	Joback Method
cpg	1216.90	J/molxK	1011.46	Joback Method
cpg	1232.55	J/molxK	1045.48	Joback Method
cpg	1247.20	J/molxK	1079.49	Joback Method
cpg	1260.91	J/molxK	1113.50	Joback Method
dvisc	0.0004557	Paxs	494.40	Joback Method
dvisc	0.0002029	Paxs	563.57	Joback Method

dvisc	0.0001078	Paxs	632.74	Joback Method
dvisc	0.0000649	Paxs	701.91	Joback Method
dvisc	0.0000428	Paxs	771.08	Joback Method
dvisc	0.0000302	Paxs	840.25	Joback Method
dvisc	0.0000225	Paxs	909.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348894&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

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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