Fumaric acid, 3-methylbut-3-enyl tetradecyl ester

Inchi: InChI=1S/C23H40O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-19-26-22(24)16-17-23(25)27-20

InchiKey: FIFVNNFPYNBJNY-WUKNDPDISA-N

Formula: C23H40O4

SMILES: C=C(C)CCOC(=O)C=CC(=O)OCCCCCCCCCCCCCCC

Mol. weight [g/mol]: 380.56

Physical Properties

Property code	Value	Unit	Source
gf	-165.55	kJ/mol	Joback Method
hf	-774.79	kJ/mol	Joback Method
hfus	58.51	kJ/mol	Joback Method
hvap	84.47	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	6.296		Crippen Method
mcvol	341.210	ml/mol	McGowan Method
pc	955.55	kPa	Joback Method
rinpol	2666.00		NIST Webbook
tb	878.94	K	Joback Method
tc	1076.27	K	Joback Method
tf	472.49	K	Joback Method
vc	1.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1099.03	J/mol×K	878.94	Joback Method
cpg	1117.52	J/mol×K	911.83	Joback Method
cpg	1134.87	J/mol×K	944.72	Joback Method
cpg	1151.13	J/mol×K	977.61	Joback Method
cpg	1166.33	J/mol×K	1010.49	Joback Method
cpg	1180.53	J/mol×K	1043.38	Joback Method
cpg	1193.76	J/mol×K	1076.27	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=U348913&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
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