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

Inchi: InChI=1S/C27H48O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-30-26(28)20-21

InchiKey: TWVYSRGLLCUDGH-QZQOTICOSA-N

Formula: C27H48O4

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

Mol. weight [g/mol]: 436.67

Physical Properties

Property code	Value	Unit	Source
gf	-131.87	kJ/mol	Joback Method
hf	-857.35	kJ/mol	Joback Method
hfus	68.87	kJ/mol	Joback Method
hvap	93.38	kJ/mol	Joback Method
log10ws	-8.56		Crippen Method
logp	7.857		Crippen Method
mcvol	397.570	ml/mol	McGowan Method
pc	763.52	kPa	Joback Method
rinpol	3070.00		NIST Webbook
rinpol	3070.00		NIST Webbook
tb	970.46	K	Joback Method
tc	1193.95	K	Joback Method
tf	517.57	K	Joback Method
vc	1.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1351.40	J/mol×K	970.46	Joback Method
cpg	1372.12	J/mol×K	1007.71	Joback Method
cpg	1391.34	J/mol×K	1044.96	Joback Method
cpg	1409.13	J/mol×K	1082.21	Joback Method
cpg	1425.58	J/mol×K	1119.46	Joback Method
cpg	1440.75	J/mol×K	1156.70	Joback Method
cpg	1454.73	J/mol×K	1193.95	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U348917&Units=SI

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