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

Inchi: InChI=1S/C28H50O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-24-31-27(29)21
InchiKey: SEYOCWWGFFRITO-QURGRASLSA-N
Formula: C28H50O4
SMILES: C=C(C)CCOC(=O)C=CC(=O)OCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 450.69

Physical Properties

Property code	Value	Unit	Source
gf	-123.45	kJ/mol	Joback Method
hf	-877.99	kJ/mol	Joback Method
hfus	71.46	kJ/mol	Joback Method
hvap	95.60	kJ/mol	Joback Method
log10ws	-8.98		Crippen Method
logp	8.247		Crippen Method
mcvol	411.660	ml/mol	McGowan Method
pc	724.57	kPa	Joback Method
rinpol	3169.00		NIST Webbook
rinpol	3169.00		NIST Webbook
tb	993.34	K	Joback Method
tc	1226.25	K	Joback Method
tf	528.84	K	Joback Method
vc	1.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1415.75	J/mol×K	993.34	Joback Method
cpg	1437.18	J/mol×K	1032.16	Joback Method
cpg	1456.97	J/mol×K	1070.98	Joback Method
cpg	1475.22	J/mol×K	1109.79	Joback Method
cpg	1492.03	J/mol×K	1148.61	Joback Method
cpg	1507.48	J/mol×K	1187.43	Joback Method
cpg	1521.67	J/mol×K	1226.25	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=U348918&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