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

Inchi: InChI=1S/C18H30O4/c1-4-5-6-7-8-9-10-14-21-17(19)11-12-18(20)22-15-13-16(2)3/h11-1
InchiKey: NZJAEXAOWGIVNB-VAWYXSNFSA-N
Formula: C18H30O4
SMILES: C=C(C)CCOC(=O)C=CC(=O)OCCCCCCCCC
Mol. weight [g/mol]: 310.43

Physical Properties

Property code	Value	Unit	Source
gf	-207.65	kJ/mol	Joback Method
hf	-671.59	kJ/mol	Joback Method
hfus	45.56	kJ/mol	Joback Method
hvap	73.34	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.346		Crippen Method
mcvol	270.760	ml/mol	McGowan Method
pc	1317.52	kPa	Joback Method
rinpol	2160.00		NIST Webbook
rinpol	2160.00		NIST Webbook
tb	764.54	K	Joback Method
tc	949.29	K	Joback Method
tf	416.14	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.03	J/mol×K	764.54	Joback Method
cpg	815.50	J/mol×K	795.33	Joback Method
cpg	831.08	J/mol×K	826.12	Joback Method
cpg	845.80	J/mol×K	856.92	Joback Method
cpg	859.68	J/mol×K	887.71	Joback Method
cpg	872.76	J/mol×K	918.50	Joback Method
cpg	885.05	J/mol×K	949.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348908&Units=SI
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

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