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

Inchi: InChI=1S/C19H32O4/c1-4-5-6-7-8-9-10-11-15-22-18(20)12-13-19(21)23-16-14-17(2)3/h1
InchiKey: MIIUAARNMOECIY-OUKQBFOZSA-N
Formula: C19H32O4
SMILES: C=C(C)CCOC(=O)C=CC(=O)OCCCCCCCCCC
Mol. weight [g/mol]: 324.45

Physical Properties

Property code	Value	Unit	Source
gf	-199.23	kJ/mol	Joback Method
hf	-692.23	kJ/mol	Joback Method
hfus	48.15	kJ/mol	Joback Method
hvap	75.57	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.736		Crippen Method
mcvol	284.850	ml/mol	McGowan Method
pc	1230.28	kPa	Joback Method
rinpol	2261.00		NIST Webbook
rinpol	2261.00		NIST Webbook
tb	787.42	K	Joback Method
tc	973.25	K	Joback Method
tf	427.41	K	Joback Method
vc	1.109	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	857.33	J/mol×K	787.42	Joback Method
cpg	874.17	J/mol×K	818.39	Joback Method
cpg	890.09	J/mol×K	849.36	Joback Method
cpg	905.11	J/mol×K	880.34	Joback Method
cpg	919.27	J/mol×K	911.31	Joback Method
cpg	932.58	J/mol×K	942.28	Joback Method
cpg	945.07	J/mol×K	973.25	Joback Method

Sources

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=U348909&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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