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

Inchi: InChI=1S/C26H46O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-29-25(27)19-20-26

InchiKey: KGPKEFQQQCDGBN-FMQUCBEESA-N

Formula: C26H46O4

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

Mol. weight [g/mol]: 422.64

Physical Properties

Property code	Value	Unit	Source
gf	-140.29	kJ/mol	Joback Method
hf	-836.71	kJ/mol	Joback Method
hfus	66.28	kJ/mol	Joback Method
hvap	91.15	kJ/mol	Joback Method
log10ws	-8.14		Crippen Method
logp	7.467		Crippen Method
mcvol	383.480	ml/mol	McGowan Method
pc	805.70	kPa	Joback Method
rinpol	2961.00		NIST Webbook
rinpol	2961.00		NIST Webbook
tb	947.58	K	Joback Method
tc	1162.90	K	Joback Method
tf	506.30	K	Joback Method
vc	1.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1287.50	J/mol×K	947.58	Joback Method
cpg	1307.59	J/mol×K	983.47	Joback Method
cpg	1326.28	J/mol×K	1019.35	Joback Method
cpg	1343.65	J/mol×K	1055.24	Joback Method
cpg	1359.75	J/mol×K	1091.13	Joback Method
cpg	1374.66	J/mol×K	1127.01	Joback Method
cpg	1388.44	J/mol×K	1162.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348916&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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