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

Inchi: InChI=1S/C25H44O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-28-24(26)18-19-25(27

InchiKey: GQHTXJIFMBTDTO-VHEBQXMUSA-N

Formula: C25H44O4

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

Mol. weight [g/mol]: 408.61

Physical Properties

Property code	Value	Unit	Source
gf	-148.71	kJ/mol	Joback Method
hf	-816.07	kJ/mol	Joback Method
hfus	63.69	kJ/mol	Joback Method
hvap	88.92	kJ/mol	Joback Method
log10ws	-7.72		Crippen Method
logp	7.076		Crippen Method
mcvol	369.390	ml/mol	McGowan Method
pc	851.47	kPa	Joback Method
rinpol	2855.00		NIST Webbook
rinpol	2855.00		NIST Webbook
tb	924.70	K	Joback Method
tc	1132.99	K	Joback Method
tf	495.03	K	Joback Method
vc	1.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1224.11	J/mol×K	924.70	Joback Method
cpg	1243.61	J/mol×K	959.41	Joback Method
cpg	1261.82	J/mol×K	994.13	Joback Method
cpg	1278.79	J/mol×K	1028.84	Joback Method
cpg	1294.58	J/mol×K	1063.56	Joback Method
cpg	1309.24	J/mol×K	1098.27	Joback Method
cpg	1322.83	J/mol×K	1132.99	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=U348915&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