Fumaric acid, 2-octyl tridec-2-yn-1-yl ester

Inchi: InChI=1S/C25H42O4/c1-4-6-8-10-11-12-13-14-15-16-18-22-28-24(26)20-21-25(27)29-23
InchiKey: QKQPEZIKBVGYQM-QZQOTICOSA-N
Formula: C25H42O4
SMILES: CCCCCCCCCCC#CCOC(=O)C=CC(=O)OC(C)CCCCCC
Mol. weight [g/mol]: 406.60

Physical Properties

Property code	Value	Unit	Source
gf	-27.64	kJ/mol	Joback Method
hf	-664.69	kJ/mol	Joback Method
hfus	65.88	kJ/mol	Joback Method
hvap	91.28	kJ/mol	Joback Method
log10ws	-7.77		Crippen Method
logp	6.522		Crippen Method
mcvol	365.090	ml/mol	McGowan Method
pc	914.94	kPa	Joback Method
rinpol	2805.00		NIST Webbook
rinpol	2805.00		NIST Webbook
tb	936.70	K	Joback Method
tc	1146.78	K	Joback Method
tf	601.85	K	Joback Method
vc	1.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1200.29	J/mol×K	936.70	Joback Method
cpg	1218.90	J/mol×K	971.71	Joback Method
cpg	1236.20	J/mol×K	1006.73	Joback Method
cpg	1252.24	J/mol×K	1041.74	Joback Method
cpg	1267.06	J/mol×K	1076.76	Joback Method
cpg	1280.72	J/mol×K	1111.77	Joback Method
cpg	1293.25	J/mol×K	1146.78	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=U405595&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