Fumaric acid, 2,4,4-trimethylpentyl tridec-2-yn-1-yl ester

Inchi: InChI=1S/C25H42O4/c1-6-7-8-9-10-11-12-13-14-15-16-19-28-23(26)17-18-24(27)29-21-

InchiKey: CWADOIYWYINDGL-ISLYRVAYSA-N

Formula: C25H42O4

SMILES: CCCCCCCCCCC#CCOC(=O)C=CC(=O)OCC(C)CC(C)(C)C

Mol. weight [g/mol]: 406.60

Physical Properties

Property code	Value	Unit	Source
gf	-24.80	kJ/mol	Joback Method
hf	-673.44	kJ/mol	Joback Method
hfus	58.47	kJ/mol	Joback Method
hvap	89.98	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	6.236		Crippen Method
mcvol	365.090	ml/mol	McGowan Method
pc	925.55	kPa	Joback Method
rinpol	2753.00		NIST Webbook
rinpol	2753.00		NIST Webbook
tb	933.47	K	Joback Method
tc	1143.55	K	Joback Method
tf	604.27	K	Joback Method
vc	1.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1200.29	J/mol×K	933.47	Joback Method
cpg	1218.81	J/mol×K	968.48	Joback Method
cpg	1236.12	J/mol×K	1003.50	Joback Method
cpg	1252.26	J/mol×K	1038.51	Joback Method
cpg	1267.32	J/mol×K	1073.52	Joback Method
cpg	1281.35	J/mol×K	1108.54	Joback Method
cpg	1294.43	J/mol×K	1143.55	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405615&Units=SI

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