Fumaric acid, 2,4,4-trimethylpentyl 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C17H28O4/c1-13(2)9-10-20-15(18)7-8-16(19)21-12-14(3)11-17(4,5)6/h7-9,14H

InchiKey: CXDHWWCAHRQJTH-BQYQJAHWSA-N

Formula: C17H28O4

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

Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-223.29	kJ/mol	Joback Method
hf	-673.19	kJ/mol	Joback Method
hfus	33.52	kJ/mol	Joback Method
hvap	70.06	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.667		Crippen Method
mcvol	256.670	ml/mol	McGowan Method
pc	1454.57	kPa	Joback Method
rinpol	1946.00		NIST Webbook
rinpol	1946.00		NIST Webbook
tb	745.47	K	Joback Method
tc	941.48	K	Joback Method
tf	388.97	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	745.40	J/mol×K	745.47	Joback Method
cpg	761.99	J/mol×K	778.14	Joback Method
cpg	777.64	J/mol×K	810.81	Joback Method
cpg	792.38	J/mol×K	843.47	Joback Method
cpg	806.26	J/mol×K	876.14	Joback Method
cpg	819.34	J/mol×K	908.81	Joback Method
cpg	831.66	J/mol×K	941.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405603&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

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