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

Inchi: InChI=1S/C17H28O4/c1-4-5-6-7-8-9-13-20-16(18)10-11-17(19)21-14-12-15(2)3/h10-11H
InchiKey: CVVXSSZKVDHVKN-ZHACJKMWSA-N
Formula: C17H28O4
SMILES: C=C(C)CCOC(=O)C=CC(=O)OCCCCCCCC
Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-216.07	kJ/mol	Joback Method
hf	-650.95	kJ/mol	Joback Method
hfus	42.97	kJ/mol	Joback Method
hvap	71.12	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.956		Crippen Method
mcvol	256.670	ml/mol	McGowan Method
pc	1414.37	kPa	Joback Method
rinpol	2065.00		NIST Webbook
rinpol	2065.00		NIST Webbook
tb	741.66	K	Joback Method
tc	925.94	K	Joback Method
tf	404.87	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.73	J/mol×K	741.66	Joback Method
cpg	757.81	J/mol×K	772.37	Joback Method
cpg	773.04	J/mol×K	803.09	Joback Method
cpg	787.44	J/mol×K	833.80	Joback Method
cpg	801.05	J/mol×K	864.51	Joback Method
cpg	813.87	J/mol×K	895.23	Joback Method
cpg	825.93	J/mol×K	925.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348907&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