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

Inchi: InChI=1S/C22H38O4/c1-4-5-6-7-8-9-10-11-12-13-14-18-25-21(23)15-16-22(24)26-19-17
InchiKey: CHDVQAZTHZAICP-FOCLMDBBSA-N
Formula: C22H38O4
SMILES: C=C(C)CCOC(=O)C=CC(=O)OCCCCCCCCCCCCC
Mol. weight [g/mol]: 366.53

Physical Properties

Property code	Value	Unit	Source
gf	-173.97	kJ/mol	Joback Method
hf	-754.15	kJ/mol	Joback Method
hfus	55.92	kJ/mol	Joback Method
hvap	82.25	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	5.906		Crippen Method
mcvol	327.120	ml/mol	McGowan Method
pc	1014.89	kPa	Joback Method
rinpol	2571.00		NIST Webbook
rinpol	2571.00		NIST Webbook
tb	856.06	K	Joback Method
tc	1049.32	K	Joback Method
tf	461.22	K	Joback Method
vc	1.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1037.46	J/mol×K	856.06	Joback Method
cpg	1055.50	J/mol×K	888.27	Joback Method
cpg	1072.47	J/mol×K	920.48	Joback Method
cpg	1088.40	J/mol×K	952.69	Joback Method
cpg	1103.33	J/mol×K	984.90	Joback Method
cpg	1117.31	J/mol×K	1017.11	Joback Method
cpg	1130.36	J/mol×K	1049.32	Joback Method

Sources

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=U348912&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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