Fumaric acid, 3,3-dimethylbut-2-yl tridecyl ester

Inchi: InChI=1S/C23H42O4/c1-6-7-8-9-10-11-12-13-14-15-16-19-26-21(24)17-18-22(25)27-20(

InchiKey: IKERNNOVPQYOLD-ISLYRVAYSA-N

Formula: C23H42O4

SMILES: CCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)(C)C

Mol. weight [g/mol]: 382.58

Physical Properties

Property code	Value	Unit	Source
gf	-244.44	kJ/mol	Joback Method
hf	-904.46	kJ/mol	Joback Method
hfus	50.16	kJ/mol	Joback Method
hvap	83.38	kJ/mol	Joback Method
log10ws	-6.90		Crippen Method
logp	6.375		Crippen Method
mcvol	345.510	ml/mol	McGowan Method
pc	943.84	kPa	Joback Method
rinpol	2542.00		NIST Webbook
rinpol	2542.00		NIST Webbook
tb	878.71	K	Joback Method
tc	1076.73	K	Joback Method
tf	475.63	K	Joback Method
vc	1.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1128.62	J/mol×K	878.71	Joback Method
cpg	1147.48	J/mol×K	911.71	Joback Method
cpg	1165.18	J/mol×K	944.72	Joback Method
cpg	1181.78	J/mol×K	977.72	Joback Method
cpg	1197.32	J/mol×K	1010.72	Joback Method
cpg	1211.86	J/mol×K	1043.72	Joback Method
cpg	1225.47	J/mol×K	1076.73	Joback Method
dvisc	0.0006051	Pa×s	475.63	Joback Method

dvisc	0.0002455	Pa×s	542.81	Joback Method
dvisc	0.0001215	Pa×s	609.99	Joback Method
dvisc	0.0000691	Pa×s	677.17	Joback Method
dvisc	0.0000435	Pa×s	744.35	Joback Method
dvisc	0.0000296	Pa×s	811.53	Joback Method
dvisc	0.0000214	Pa×s	878.71	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=U348712&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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

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