Fumaric acid, 2-methylpentyl tetradecyl ester

Inchi: InChI=1S/C24H44O4/c1-4-6-7-8-9-10-11-12-13-14-15-16-20-27-23(25)18-19-24(26)28-2
InchiKey: ODYQLNFDSKFJTI-VHEBQXMUSA-N
Formula: C24H44O4
SMILES: CCCCCCCCCCCCCCOC(=O)C=CC(=O)OCC(C)CCC
Mol. weight [g/mol]: 396.60

Physical Properties

Property code	Value	Unit	Source
gf	-238.86	kJ/mol	Joback Method
hf	-916.35	kJ/mol	Joback Method
hfus	60.17	kJ/mol	Joback Method
hvap	86.90	kJ/mol	Joback Method
log10ws	-7.21		Crippen Method
logp	6.766		Crippen Method
mcvol	359.600	ml/mol	McGowan Method
pc	880.52	kPa	Joback Method
rinpol	2671.00		NIST Webbook
tb	904.82	K	Joback Method
tc	1108.02	K	Joback Method
tf	484.48	K	Joback Method
vc	1.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1190.97	J/mol×K	904.82	Joback Method
cpg	1210.47	J/mol×K	938.69	Joback Method
cpg	1228.67	J/mol×K	972.55	Joback Method
cpg	1245.63	J/mol×K	1006.42	Joback Method
cpg	1261.38	J/mol×K	1040.29	Joback Method
cpg	1275.97	J/mol×K	1074.15	Joback Method
cpg	1289.45	J/mol×K	1108.02	Joback Method
dvisc	0.0005674	Pa×s	484.48	Joback Method
dvisc	0.0002387	Pa×s	554.54	Joback Method

dvisc	0.0001219	Pa×s	624.59	Joback Method
dvisc	0.0000713	Pa×s	694.65	Joback Method
dvisc	0.0000460	Pa×s	764.71	Joback Method
dvisc	0.0000320	Pa×s	834.76	Joback Method
dvisc	0.0000235	Pa×s	904.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348732&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
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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