Fumaric acid, 4-methylpent-2-yl pentadecyl ester

Inchi: InChI=1S/C25H46O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-20-28-24(26)18-19-25(27)2
InchiKey: INFVEGCLOQCEGF-VHEBQXMUSA-N
Formula: C25H46O4
SMILES: CCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)CC(C)C
Mol. weight [g/mol]: 410.63

Physical Properties

Property code	Value	Unit	Source
gf	-232.88	kJ/mol	Joback Method
hf	-942.27	kJ/mol	Joback Method
hfus	59.24	kJ/mol	Joback Method
hvap	88.74	kJ/mol	Joback Method
log10ws	-7.74		Crippen Method
logp	7.155		Crippen Method
mcvol	373.690	ml/mol	McGowan Method
pc	836.28	kPa	Joback Method
rinpol	2744.00		NIST Webbook
rinpol	2744.00		NIST Webbook
tb	927.26	K	Joback Method
tc	1136.14	K	Joback Method
tf	480.75	K	Joback Method
vc	1.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1254.59	J/mol×K	927.26	Joback Method
cpg	1274.51	J/mol×K	962.07	Joback Method
cpg	1293.04	J/mol×K	996.89	Joback Method
cpg	1310.23	J/mol×K	1031.70	Joback Method
cpg	1326.13	J/mol×K	1066.51	Joback Method
cpg	1340.79	J/mol×K	1101.32	Joback Method
cpg	1354.26	J/mol×K	1136.14	Joback Method
dvisc	0.0005844	Pa×s	480.75	Joback Method

dvisc	0.0002231	Pa×s	555.17	Joback Method
dvisc	0.0001070	Pa×s	629.59	Joback Method
dvisc	0.0000599	Pa×s	704.00	Joback Method
dvisc	0.0000375	Pa×s	778.42	Joback Method
dvisc	0.0000255	Pa×s	852.84	Joback Method
dvisc	0.0000184	Pa×s	927.26	Joback Method

Sources

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=U348329&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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