Fumaric acid, 2-hexyl pentadecyl ester

Inchi: InChI=1S/C25H46O4/c1-4-6-8-9-10-11-12-13-14-15-16-17-18-22-28-24(26)20-21-25(27)29-23(5-2)19-7-3/h20-21,23H,4-19,22H2,1-3H3/b21-20+

InchiKey: SPUIBFUZZXSFKO-QZQOTICOSA-N

Formula: C25H46O4

SMILES: CCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)CCCC

Mol. weight [g/mol]: 410.63

Physical Properties

Property code	Value	Unit	Source
gf	-230.44	kJ/mol	Joback Method
hf	-936.99	kJ/mol	Joback Method
hfus	62.76	kJ/mol	Joback Method
hvap	89.13	kJ/mol	Joback Method
log10ws	-7.98		Crippen Method
logp	7.299		Crippen Method
mcvol	373.690	ml/mol	McGowan Method
pc	832.42	kPa	Joback Method
rinpol	2790.00		NIST Webbook
rinpol	2790.00		NIST Webbook
tb	927.70	K	Joback Method
tc	1137.27	K	Joback Method
tf	495.75	K	Joback Method
vc	1.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1254.19	J/mol×K	927.70	Joback Method
cpg	1340.92	J/mol×K	1102.34	Joback Method
cpg	1326.14	J/mol×K	1067.41	Joback Method
cpg	1310.14	J/mol×K	1032.49	Joback Method
cpg	1292.84	J/mol×K	997.56	Joback Method
cpg	1274.21	J/mol×K	962.63	Joback Method
cpg	1354.51	J/mol×K	1137.27	Joback Method
dvisc	0.0000202	Pa×s	927.70	Joback Method

dvisc	0.0000275	Pa×s	855.71	Joback Method
dvisc	0.0000396	Pa×s	783.72	Joback Method
dvisc	0.0000616	Pa×s	711.72	Joback Method
dvisc	0.0001057	Pa×s	639.73	Joback Method
dvisc	0.0002080	Pa×s	567.74	Joback Method
dvisc	0.0004981	Pa×s	495.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348753&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