Fumaric acid, hexadecyl pent-4-enyl ester

Inchi: InChI=1S/C25H44O4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-19-23-29-25(27)21-20-24(2
InchiKey: VLNKWXUIAJGQCF-QZQOTICOSA-N
Formula: C25H44O4
SMILES: C=CCCCOC(=O)C=CC(=O)OCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 408.61

Physical Properties

Property code	Value	Unit	Source
gf	-140.16	kJ/mol	Joback Method
hf	-806.28	kJ/mol	Joback Method
hfus	65.00	kJ/mol	Joback Method
hvap	88.84	kJ/mol	Joback Method
log10ws	-7.72		Crippen Method
logp	7.076		Crippen Method
mcvol	369.390	ml/mol	McGowan Method
pc	849.00	kPa	Joback Method
rinpol	2870.00		NIST Webbook
rinpol	2870.00		NIST Webbook
tb	924.82	K	Joback Method
tc	1133.61	K	Joback Method
tf	508.99	K	Joback Method
vc	1.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1224.49	J/mol×K	924.82	Joback Method
cpg	1309.63	J/mol×K	1098.81	Joback Method
cpg	1294.99	J/mol×K	1064.01	Joback Method
cpg	1279.21	J/mol×K	1029.21	Joback Method
cpg	1262.24	J/mol×K	994.42	Joback Method
cpg	1244.02	J/mol×K	959.62	Joback Method
cpg	1323.18	J/mol×K	1133.61	Joback Method
dvisc	0.0000238	Pa×s	924.82	Joback Method

dvisc	0.0000318	Pa×s	855.52	Joback Method
dvisc	0.0000447	Pa×s	786.21	Joback Method
dvisc	0.0000672	Pa×s	716.90	Joback Method
dvisc	0.0001102	Pa×s	647.60	Joback Method
dvisc	0.0002035	Pa×s	578.29	Joback Method
dvisc	0.0004438	Pa×s	508.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348856&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