

Fumaric acid, hexadecyl 3-hexyl ester

Inchi:	InChI=1S/C26H48O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-23-29-25(27)21-22-26(
InchiKey:	FLSGKPQRSNUFHV-QURGRASLSA-N
Formula:	C26H48O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(CC)CCC
Mol. weight [g/mol]:	424.66

Physical Properties

Property code	Value	Unit	Source
gf	-222.02	kJ/mol	Joback Method
hf	-957.63	kJ/mol	Joback Method
hfus	65.35	kJ/mol	Joback Method
hvap	91.35	kJ/mol	Joback Method
log10ws	-8.40		Crippen Method
logp	7.689		Crippen Method
mcvol	387.780	ml/mol	McGowan Method
pc	788.16	kPa	Joback Method
rinpol	2906.00		NIST Webbook
tb	950.58	K	Joback Method
tc	1167.61	K	Joback Method
tf	507.02	K	Joback Method
vc	1.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1317.93	J/molxK	950.58	Joback Method
cpg	1338.52	J/molxK	986.75	Joback Method
cpg	1357.62	J/molxK	1022.92	Joback Method
cpg	1375.27	J/molxK	1059.10	Joback Method
cpg	1391.54	J/molxK	1095.27	Joback Method
cpg	1406.49	J/molxK	1131.44	Joback Method
cpg	1420.19	J/molxK	1167.61	Joback Method
dvisc	0.0004362	Paxs	507.02	Joback Method
dvisc	0.0001808	Paxs	580.95	Joback Method

dvisc	0.0000914	Paxs	654.87	Joback Method
dvisc	0.0000531	Paxs	728.80	Joback Method
dvisc	0.0000341	Paxs	802.73	Joback Method
dvisc	0.0000236	Paxs	876.65	Joback Method
dvisc	0.0000173	Paxs	950.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348614&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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