

Fumaric acid, cis-hex-3-enyl hexadecyl ester

Inchi:	InChI=1S/C26H46O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-20-24-30-26(28)22-21-25(
InchiKey:	ZJPWZNLKZXPKHJ-RDVPLAOUA-N
Formula:	C26H46O4
SMILES:	CCC=CCCOC(=O)C=CC(=O)OCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	422.64

Physical Properties

Property code	Value	Unit	Source
gf	-139.36	kJ/mol	Joback Method
hf	-835.13	kJ/mol	Joback Method
hfus	69.07	kJ/mol	Joback Method
hvap	91.70	kJ/mol	Joback Method
log10ws	-8.14		Crippen Method
logp	7.467		Crippen Method
mcvol	383.480	ml/mol	McGowan Method
pc	807.99	kPa	Joback Method
rinqol	2991.00		NIST Webbook
tb	955.18	K	Joback Method
tc	1172.59	K	Joback Method
tf	516.94	K	Joback Method
vc	1.500	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1289.79	J/molxK	955.18	Joback Method
cpg	1309.98	J/molxK	991.42	Joback Method
cpg	1328.84	J/molxK	1027.65	Joback Method
cpg	1346.43	J/molxK	1063.89	Joback Method
cpg	1362.84	J/molxK	1100.12	Joback Method
cpg	1378.13	J/molxK	1136.36	Joback Method
cpg	1392.39	J/molxK	1172.59	Joback Method
dvisc	0.0003540	Paxs	516.94	Joback Method
dvisc	0.0001550	Paxs	589.98	Joback Method

dvisc	0.0000814	Paxs	663.02	Joback Method
dvisc	0.0000486	Paxs	736.06	Joback Method
dvisc	0.0000319	Paxs	809.10	Joback Method
dvisc	0.0000224	Paxs	882.14	Joback Method
dvisc	0.0000166	Paxs	955.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348871&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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