

Fumaric acid, di(1-methoxydec-4-yl) ester

Inchi:	InChI=1S/C26H48O6/c1-5-7-9-11-15-23(17-13-21-29-3)31-25(27)19-20-26(28)32-24(18-
InchiKey:	MNMSJWVXTDFPFZ-FMQUCBEESA-N
Formula:	C26H48O6
SMILES:	CCCCCCC(CCCOC)OC(=O)C=CC(=O)OC(CCCCCC)CCOC
Mol. weight [g/mol]:	456.66

Physical Properties

Property code	Value	Unit	Source
gf	-434.46	kJ/mol	Joback Method
hf	-1227.35	kJ/mol	Joback Method
hfus	64.20	kJ/mol	Joback Method
hvap	95.78	kJ/mol	Joback Method
log10ws	-6.68		Crippen Method
logp	6.160		Crippen Method
mvol	399.520	ml/mol	McGowan Method
pc	776.77	kPa	Joback Method
rinpol	2889.00		NIST Webbook
tb	994.98	K	Joback Method
tc	1227.30	K	Joback Method
tf	536.48	K	Joback Method
vc	1.544	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1380.60	J/molxK	994.98	Joback Method
cpg	1399.99	J/molxK	1033.70	Joback Method
cpg	1417.38	J/molxK	1072.42	Joback Method
cpg	1432.80	J/molxK	1111.14	Joback Method
cpg	1446.31	J/molxK	1149.86	Joback Method
cpg	1457.92	J/molxK	1188.58	Joback Method
cpg	1467.69	J/molxK	1227.30	Joback Method
dvisc	0.0002193	Paxs	536.48	Joback Method
dvisc	0.0000908	Paxs	612.90	Joback Method

dvisc	0.0000458	Paxs	689.31	Joback Method
dvisc	0.0000264	Paxs	765.73	Joback Method
dvisc	0.0000169	Paxs	842.15	Joback Method
dvisc	0.0000116	Paxs	918.56	Joback Method
dvisc	0.0000084	Paxs	994.98	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405909&Units=SI

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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