

Fumaric acid, di(2-(2-methoxyethyl)hexyl)ester

Inchi:	InChI=1S/C22H40O6/c1-5-7-9-19(13-15-25-3)17-27-21(23)11-12-22(24)28-18-20(10-8-6
InchiKey:	MVFJAKQKABCLEN-VAWYXSNFSA-N
Formula:	C22H40O6
SMILES:	CCCCC(CCOC)COC(=O)C=CC(=O)OCC(CCCC)CCOC
Mol. weight [g/mol]:	400.55

Physical Properties

Property code	Value	Unit	Source
gf	-468.14	kJ/mol	Joback Method
hf	-1144.79	kJ/mol	Joback Method
hfus	53.84	kJ/mol	Joback Method
hvap	86.88	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	4.315		Crippen Method
mcvol	343.160	ml/mol	McGowan Method
pc	974.13	kPa	Joback Method
rinpol	2607.00		NIST Webbook
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tb	903.46	K	Joback Method
tc	1106.10	K	Joback Method
tf	491.40	K	Joback Method
vc	1.319	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1129.44	J/molxK	903.46	Joback Method
cpg	1147.33	J/molxK	937.23	Joback Method
cpg	1163.82	J/molxK	971.01	Joback Method
cpg	1178.91	J/molxK	1004.78	Joback Method
cpg	1192.64	J/molxK	1038.55	Joback Method
cpg	1205.01	J/molxK	1072.32	Joback Method
cpg	1216.03	J/molxK	1106.10	Joback Method
dvisc	0.0003788	Paxs	491.40	Joback Method

dvisc	0.0001616	Paxs	560.08	Joback Method
dvisc	0.0000830	Paxs	628.75	Joback Method
dvisc	0.0000486	Paxs	697.43	Joback Method
dvisc	0.0000314	Paxs	766.11	Joback Method
dvisc	0.0000217	Paxs	834.78	Joback Method
dvisc	0.0000159	Paxs	903.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405895&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
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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