Fumaric acid, di(3-(2-methoxyethyl)heptyl) ester

Inchi: InChI=1S/C25H46O6/c1-5-7-10-22(15-19-28-3)12-9-18-30-24(26)13-14-25(27)31-21-17-

InchiKey: NHSWDKGMJMKYTM-BUHFOSPRSA-N

Formula: C25H46O6

SMILES: CCCCC(CCCOC(=O)C=CC(=O)OCCC(CCCC)CCOC)CCOC

Mol. weight [g/mol]: 442.63

Physical Properties

Property code	Value	Unit	Source
gf	-442.88	kJ/mol	Joback Method
hf	-1206.71	kJ/mol	Joback Method
hfus	61.61	kJ/mol	Joback Method
hvap	93.56	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	5.485		Crippen Method
mcvol	385.430	ml/mol	McGowan Method
pc	820.07	kPa	Joback Method
rinpol	2836.00		NIST Webbook
rinpol	2836.00		NIST Webbook
tb	972.10	K	Joback Method
tc	1195.25	K	Joback Method
tf	525.21	K	Joback Method
vc	1.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1317.22	J/mol×K	972.10	Joback Method
cpg	1336.21	J/mol×K	1009.29	Joback Method
cpg	1353.38	J/mol×K	1046.48	Joback Method
cpg	1368.76	J/mol×K	1083.68	Joback Method
cpg	1382.39	J/mol×K	1120.87	Joback Method
cpg	1394.29	J/mol×K	1158.06	Joback Method
cpg	1404.49	J/mol×K	1195.25	Joback Method
dvisc	0.0002523	Pa×s	525.21	Joback Method

dvisc	0.0001052	Pa×s	599.69	Joback Method
dvisc	0.0000533	Pa×s	674.17	Joback Method
dvisc	0.0000309	Pa×s	748.65	Joback Method
dvisc	0.0000197	Pa×s	823.14	Joback Method
dvisc	0.0000136	Pa×s	897.62	Joback Method
dvisc	0.0000099	Pa×s	972.10	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405911&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