Sebacic acid, heptyl 2-(2-methoxyethyl)heptyl ester

Inchi: InChI=1S/C27H52O5/c1-4-6-8-13-17-22-31-26(28)19-15-11-9-10-12-16-20-27(29)32-24-
InchiKey: KVQROMPFRMUMGR-UHFFFAOYSA-N
Formula: C27H52O5
SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)OCC(CCCCC)CCOC
Mol. weight [g/mol]: 456.70

Physical Properties

Property code	Value	Unit	Source
gf	-398.82	kJ/mol	Joback Method
hf	-1227.71	kJ/mol	Joback Method
hfus	68.92	kJ/mol	Joback Method
hvap	96.03	kJ/mol	Joback Method
log10ws	-7.70		Crippen Method
logp	7.397		Crippen Method
mcvol	412.040	ml/mol	McGowan Method
pc	719.91	kPa	Joback Method
rinpol	3115.00		NIST Webbook
rinpol	3115.00		NIST Webbook
tb	991.72	K	Joback Method
tc	1229.04	K	Joback Method
tf	545.60	K	Joback Method
vc	1.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1441.72	J/mol×K	991.72	Joback Method
cpg	1527.37	J/mol×K	1189.49	Joback Method
cpg	1514.33	J/mol×K	1149.93	Joback Method
cpg	1499.30	J/mol×K	1110.38	Joback Method
cpg	1482.22	J/mol×K	1070.83	Joback Method
cpg	1463.04	J/mol×K	1031.27	Joback Method
cpg	1538.45	J/mol×K	1229.04	Joback Method
dvisc	0.0000123	Pa×s	991.72	Joback Method

dvisc	0.0000167	Pa×s	917.37	Joback Method
dvisc	0.0000240	Pa×s	843.01	Joback Method
dvisc	0.0000369	Pa×s	768.66	Joback Method
dvisc	0.0000622	Pa×s	694.31	Joback Method
dvisc	0.0001189	Pa×s	619.95	Joback Method
dvisc	0.0002711	Pa×s	545.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354356&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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