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

Inchi: InChI=1S/C24H46O5/c1-5-6-11-14-22(17-18-27-4)20-29-24(26)16-13-10-8-7-9-12-15-23

InchiKey: KEMIPQUGRUZJIU-UHFFFAOYSA-N

Formula: C24H46O5

SMILES: CCCCCC(CCOC)COC(=O)CCCCCCCCC(=O)OCC(C)C

Mol. weight [g/mol]: 414.62

Physical Properties

Property code	Value	Unit	Source
gf	-426.52	kJ/mol	Joback Method
hf	-1171.07	kJ/mol	Joback Method
hfus	57.63	kJ/mol	Joback Method
hvap	88.96	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	6.083		Crippen Method
mcvol	369.770	ml/mol	McGowan Method
pc	849.49	kPa	Joback Method
rinpol	2764.00		NIST Webbook
rinpol	2764.00		NIST Webbook
tb	922.64	K	Joback Method
tc	1131.32	K	Joback Method
tf	496.79	K	Joback Method
vc	1.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1250.53	J/mol×K	922.64	Joback Method
cpg	1270.20	J/mol×K	957.42	Joback Method
cpg	1288.29	J/mol×K	992.20	Joback Method
cpg	1304.80	J/mol×K	1026.98	Joback Method
cpg	1319.78	J/mol×K	1061.76	Joback Method
cpg	1333.23	J/mol×K	1096.54	Joback Method
cpg	1345.19	J/mol×K	1131.32	Joback Method
dvisc	0.0004693	Pa×s	496.79	Joback Method

dvisc	0.0001943	Pa×s	567.76	Joback Method
dvisc	0.0000979	Pa×s	638.74	Joback Method
dvisc	0.0000565	Pa×s	709.71	Joback Method
dvisc	0.0000361	Pa×s	780.69	Joback Method
dvisc	0.0000248	Pa×s	851.66	Joback Method
dvisc	0.0000181	Pa×s	922.64	Joback Method

Sources

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=U354351&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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