

Sebacic acid, heptyl 2-methoxybenzyl ester

Inchi: InChI=1S/C25H40O5/c1-3-4-5-10-15-20-29-24(26)18-11-8-6-7-9-12-19-25(27)30-21-22-
InchiKey: JVYKDTIHPVQWCW-UHFFFAOYSA-N
Formula: C25H40O5
SMILES: CCCCCCOC(=O)CCCCCCCC(=O)OCc1cccc1OC
Mol. weight [g/mol]: 420.58

Physical Properties

Property code	Value	Unit	Source
gf	-310.44	kJ/mol	Joback Method
hf	-956.09	kJ/mol	Joback Method
hfus	60.92	kJ/mol	Joback Method
hvap	94.90	kJ/mol	Joback Method
log10ws	-7.31		Crippen Method
logp	6.373		Crippen Method
mvol	360.100	ml/mol	McGowan Method
pc	960.29	kPa	Joback Method
rinpol	3083.00		NIST Webbook
rinpol	3083.00		NIST Webbook
tb	978.06	K	Joback Method
tc	1197.84	K	Joback Method
tf	577.00	K	Joback Method
vc	1.393	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1210.94	J/molxK	978.06	Joback Method
cpg	1277.74	J/molxK	1161.21	Joback Method
cpg	1267.54	J/molxK	1124.58	Joback Method
cpg	1255.79	J/molxK	1087.95	Joback Method
cpg	1242.47	J/molxK	1051.32	Joback Method
cpg	1227.53	J/molxK	1014.69	Joback Method
cpg	1286.41	J/molxK	1197.84	Joback Method
dvisc	0.0000196	Paxs	978.06	Joback Method

dvisc	0.0000255	Paxs	911.22	Joback Method
dvisc	0.0000345	Paxs	844.37	Joback Method
dvisc	0.0000493	Paxs	777.53	Joback Method
dvisc	0.0000754	Paxs	710.69	Joback Method
dvisc	0.0001258	Paxs	643.84	Joback Method
dvisc	0.0002363	Paxs	577.00	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=U380776&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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