

Sebacic acid, 2,4-dimethylpent-3-yl isoheptyl ester

Inchi:	InChI=1S/C23H44O4/c1-18(2)14-13-17-26-21(24)15-11-9-7-8-10-12-16-22(25)27-23(19)
InchiKey:	DUCOCKOBWLTADG-UHFFFAOYSA-N
Formula:	C23H44O4
SMILES:	CC(C)CCCOC(=O)CCCCCCCC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]:	384.59

Physical Properties

Property code	Value	Unit	Source
gf	-334.82	kJ/mol	Joback Method
hf	-1028.77	kJ/mol	Joback Method
hfus	46.81	kJ/mol	Joback Method
hvap	83.55	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	6.310		Crippen Method
mvol	349.810	ml/mol	McGowan Method
pc	917.16	kPa	Joback Method
rinpol	2500.00		NIST Webbook
tb	876.46	K	Joback Method
tc	1073.32	K	Joback Method
tf	433.29	K	Joback Method
vc	1.347	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1156.28	J/molxK	876.46	Joback Method
cpg	1175.85	J/molxK	909.27	Joback Method
cpg	1194.08	J/molxK	942.08	Joback Method
cpg	1211.02	J/molxK	974.89	Joback Method
cpg	1226.67	J/molxK	1007.70	Joback Method
cpg	1241.08	J/molxK	1040.51	Joback Method
cpg	1254.27	J/molxK	1073.32	Joback Method
dvisc	0.0012150	Paxs	433.29	Joback Method
dvisc	0.0003922	Paxs	507.15	Joback Method

dvisc	0.0001688	Paxs	581.01	Joback Method
dvisc	0.0000878	Paxs	654.88	Joback Method
dvisc	0.0000522	Paxs	728.74	Joback Method
dvisc	0.0000341	Paxs	802.60	Joback Method
dvisc	0.0000240	Paxs	876.46	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=U355428&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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